DEVELOPMENT AND CALIBRATION OF THE THREE-DIMENSIONAL SITE-SCALE UNSATURATED ZONE MODEL OF YUCCA MOUNTAIN, NEVADA

EDITED BY:

G.S. BODVARSSON
AND
T.M. BANDURRAGA

AUGUST 1996

ERNEST ORLANDO LAWRENCE
BERKELEY NATIONAL LABORATORY

EARTH SCIENCES DIVISION

Table of Contents

CHAPTER 1:

DEVELOPMENT OF THE UNSATURATED ZONE MODEL IN FISCAL YEAR 1996

G.S. BODVARSSON, T.M. BANDURRAGA, AND Y.S. WU1

1.0 Introduction2

1.1 Conceptual Model of the UZ4

1.1.1 Conceptual Model Development 4

1.1.2 Geological Framework5

1.1.3 Infiltration6

1.1.4 Percolation Flux 7

1.1.5 Lateral Flow8

1.1.6 Effects of Major Faults8

1.1.7 Perched Water9

1.1.8 The Effect of Zeolites on Repository to Water Table Flow Paths10

1.1.9 Fluid (Water and Gas) Flow Paths and Ages13

1.1.10 Geothermal Gradient13

1.2 UZ Model and Work Elements in FY9614

1.2.1 Geology and the Numerical Grid 14

1.2.2 Initial and Boundary Conditions; Model Assumptions15

1.2.3 Rock Properties15

1.2.4 Computer Codes and Numerical Approaches16

1.2.5 Model Calibration Activities16

1.2.6 Coupled Process Calibrations and Analysis17

1.2.7 Sensitivity Analyses17

Table of Contents

1.2.8 Model Predictions	17
1.2.9 Model Uses and Limitations	18
1.3 Summary and Conclusion of FY96 Work	19
1.3.1 Percolation Flux	20
1.3.2 Lateral Flow in the Unsaturated Zone	20
1.3.3 Effects of Major Faults	21
1.3.4 Fast Flow Paths	21
1.3.5 Perched Water	22
1.3.6 Evaluation of Calibration Quality of the UZ Model	22
1.3.7 Thermal Loading Studies	23
1.3.8 Climate Change Scenario	23
1.4 Acknowledgments	23
1.5 References	24
<hr/>	
CHAPTER 2:	
GEOLOGICAL MODEL DEVELOPMENT AND VERTICAL LAYERING SCHEME FOR THE NUMERICAL GRID	
T.M. BANDURRAGA	31
<hr/>	
2.1 Introduction	32
2.1.1 QA status of data and software used in this chapter	33
2.2 Extended Model Domain	34
2.3 Vertical Layer Subdivision	36
2.3.1 Gas pressure measurements and modeling results	40
2.3.2 Borehole data measurements	40
2.3.3 Report Evaluation	43
2.3.4 Grid Discretization Studies	45
2.4 Sublayer Selections	45
2.4.1 TCw Sublayers	46

Table of Contents

2.4.2 PTn Sublayers	48
2.4.3 TSw Sublayers	49
2.4.4 CHn and CFu Sublayers	50
2.4.5 Water Table	52
2.5 Summary and Conclusions	54
2.5.1 Summary	54
2.5.2 Conclusions	54
2.5.3 Future Work	54
2.6 References	55
References for Borehole Lithostratigraphic Contacts	57

CHAPTER 3:

SATURATION AND CAPILLARY PRESSURE ANALYSIS

T. M. BANDURRAGA, S. FINSTERLE, AND G.S. BODVARSSON	62
---	----

3.1 Introduction	63
3.1.1 UZ Model Calibration	63
3.1.2 Saturation and Capillary Pressure Use and Limitations	64
3.1.3 Objectives of Saturation and Capillary Pressure Calibration	64
3.1.4 Previous Work	64
3.1.5 Model Calibration Issues	65
3.1.6 Chapter Organization	66
3.2 Data Description	66
3.2.1 Available Borehole and Fracture Data	66
3.2.2 Matrix and Fracture Hydrogeologic Parameters	68
3.3 Calibration Methodology	74
3.3.1 Development of Submodel	74
3.3.2 Conceptual Model	74

Table of Contents

3.3.3 Inversion Code and Formulating the Inverse Problem	76
3.3.4 Parameter Sensitivity Selection	77
3.3.5 Formulation of Submodel and Calibration Methodology	77
3.4 Combined Column Inversions, Uniform Infiltration Rates	79
3.4.1 Uniform Infiltration Rates	79
3.4.2 Combined Column Inversion Approach	79
3.4.3 Combined Column Results, 0.1 mm/yr Uniform Infiltration Rate	80
3.4.4 Combined Column Results, All Uniform Infiltration Rates	89
3.5 Sensitivity Studies	105
3.5.1 Spatially Variable Infiltration Rates	105
3.5.2 Spatially Varying Parameter Distributions	106
3.5.3 Coupled Permeability and van Genuchten Alpha Parameter Study	112
3.5.4 Borehole Water Potential Measurements	118
3.5.5 Effects of Sensitivity Limit and Prior Data	120
3.5.6 Additional Work	122
3.6 Conclusion	122
3.6.1 Q Status of Study	122
3.6.2 Conclusions	123
3.6.3 Future Work	126
3.7 References	127

CHAPTER 4:

COMPUTER MODELS AND THEIR DEVELOPMENT FOR THE UNSATURATED ZONE MODEL AT YUCCA MOUNTAIN Y.S. WU, S. FINSTERLE, AND K. PRUESS

4.1 Introduction	132
4.2 TOUGH2 Code	133
4.2.1 Mathematical Formulation of Mass and Energy Balance	134

Table of Contents

4.2.2 Numerical Scheme - IFD	137
4.2.3 Options of EOS Modules	139
4.2.4 Boundary Condition Treatment	141
4.2.5 Treatment of Fractured/Matrix Flow and Interaction	142
4.3 ITOUGH2	145
4.3.1 Introduction	145
4.3.2 Methodology	147
4.3.3 Applicability of ITOUGH2	153
4.4 Rautman's Thermal Conductivity Model	154
4.5 Effective Continuum Approach	154
4.5.1 Generalized Effective Continuum Approach	155
4.5.2 Threshold Saturation Fracture Flow ECM Formulation	158
4.6 Discussion of Modeling Issues	161
4.6.1 Weighting Scheme for Mobilities	161
4.6.2 Treatment of Fracture and Matrix Flow	162
4.7 Gas Flow Module	163
4.8 Radionuclide Transport Module	164
4.9 References	165
<hr/>	
CHAPTER 5:	
GRID GENERATION AND ANALYSIS	
C. HAUKWA AND G. CHEN	169
<hr/>	
5.1 Introduction	170
5.2 Development Of Mesh Generator For Complex Geometry	170
5.2.1 Input Data Structure	171
5.2.2 Code Description	172
5.2.3 Mesh Validation	173

Table of Contents

5.2.4 Future Work	173
5.2.5 Summary	174
5.3 Development Of the 3-D Site Scale Model Grid Of Yucca Mountain	174
5.3.1 2-D Areal extent of the FY96 UZ Model Grid	175
5.3.2 2-D Areal Extent of the Gas Effects Grid	176
5.3.3 Criteria for 2-D Grids	177
5.3.4 Development of the 3-D Numerical Grids	178
5.3.5 Summary	181
5.4 Grid Sensitivity Analysis in Numerical Modeling of the Unsaturated Zone	181
5.4.1 Design of Refined Grids	182
5.4.2 Results of Numerical Simulations	183
5.4.3 Summary	186
5.5 References	189

CHAPTER 6:

INVESTIGATION OF CONCEPTUAL AND NUMERICAL APPROACHES FOR EVALUATING GAS, MOISTURE, HEAT AND CHEMICAL TRANSPORT

C. DOUGHTY AND G.S. BODVARSSON	190
--------------------------------------	-----

6.1 Introduction	191
6.2 QA Status of Data and Software used in this Chapter	192
6.3 Numerical Formulations	192
6.3.1 Single-Continuum Models	193
6.3.2 Effective-Continuum Models	193
6.3.3 Dual-Continua Models	194
6.4 Conceptual Model Considered	196
6.4.1 Vertical Column Selected	196
6.4.2 Properties and Boundary Conditions	197

Table of Contents

6.5 Numerical Comparative Studies.....	198
6.5.1 Steady-State Moisture Flow	198
6.5.2 Transient Moisture flow	203
6.5.3 Transient Gas Flow	211
6.5.4 Tracer Transport	214
6.5.5 Thermal loading	219
6.6 Summary and Conclusions	227
6.6.1 Comparison of Physical-Process Representation	228
6.6.2 Comparison of Numerical Performance	228
6.7 References.....	230

CHAPTER 7:

PERCHED WATER ANALYSIS

Y.WS. WU, G. CHEN, AND G.S. BODVARSSON	232
--	-----

7.1 Introduction.....	233
7.2 QA Status of Data and Software	234
7.3 Perched Water Data.....	235
7.3.1 Borehole Perched Water Data	236
7.3.2 Chemistry and Ages of Perched Water	238
7.4 Conceptual Model.....	239
7.5 Development of the Perched Water Model	242
7.5.1 Modeling Approach and Model Description	242
7.5.2 Boundary Conditions and Model Parameters	244
7.5.3 Results and Analyses	249
7.6 Current Studies Using the New Infiltration Map.....	266
7.7 Conclusions	266
7.8 References.....	268

Table of Contents

CHAPTER 8:

THREE-DIMENSIONAL MODEL CALIBRATION AND SENSITIVITY STUDIES

Y.S. WU, G. CHEN, C. HAUKWA, AND G. S. BODVARSSON271

8.1 Introduction	272
8.2 QA Status of Data and Computer Software	274
8.3 Model Description.....	276
8.3.1 Model Domain and Grid	276
8.3.2 Modeling Approach	277
8.3.3 Model Boundary Conditions.....	279
8.4 Implementation of Different Infiltration Maps.....	282
8.5 Model Parameters and Rock Properties.....	284
8.5.1 Parameter Set # 1	285
8.5.2 Parameter Set # 2	287
8.5.3 Parameter Set # 3	288
8.5.4 Parameter Set # 4	289
8.5.5 Rock Name and Specification	290
8.5.6 Fault Properties.....	291
8.6 Comparisons with Observed Borehole Data.....	293
8.6.1 Comparisons with UZ-1/14 Data	293
8.6.2 Comparisons with NRG-7a Data	294
8.6.3 Comparisons with SD-7 Data	295
8.6.4 Comparisons with SD-9 Data	296
8.6.5 Comparisons with SD-12 Data	297
8.6.6 Comparisons with UZ#16 Data	298
8.6.7 Comparisons with NRG-6 Data	299
8.7 Effects of Rock Property Variations on Moisture and Heat Flow	300

Table of Contents

8.7.1 Lateral Moisture Movement and Distribution in Selected 2-D Vertical Cross Sections	300
8.7.2 3-D Lateral Moisture Distributions and Movement	313
8.7.3 Ambient Geothermal Conditions and Heat Flow at Repository Horizon	320
8.8 Effects of Fault Properties	322
8.8.1 W-E Cross Section at SD-7	323
8.8.2 W-E Cross Section at UZ-1/14	327
8.8.3 Groundwater Travel Times	330
8.9 3-D Dual-Permeability Model	330
8.9.1 Dual-Permeability Model Grid and Parameters	330
8.9.2 Comparisons with the ECM Results	331
8.9.3 Effects of Climate Changes Using High-Pulse Infiltration	333
8.10 Simulations of Percolation Fluxes	338
8.10.1 Percolation Fluxes at Repository Horizon	338
8.10.2 Water Recharge Maps at the Water Table	343
8.11 Summary, Conclusions and Recommendations	348
8.11.1 Summary	348
8.11.2 Conclusions	348
8.11.3 Recommendations	350
8.12 References	350
<hr/>	
CHAPTER 9:	
TEMPERATURE AND HEAT FLOW ANALYSIS	
<i>G.S. BODVARSSON, Y.S. WU, AND S. FINSTERLE</i>	355
<hr/>	
9.1 Introduction	356
9.2 QA Status of Data and Software Used in this Chapter	357
9.3 Temperature and Heat Flow Data	358
9.3.1 Temperature Data	358

Table of Contents

9.3.2 Heat Flow Data	364
9.4 Heat Conduction Analysis.....	366
9.4.1 Model Description	366
9.4.2 Model Parameters And Boundary Conditions	366
9.4.3 Simulation And Comparison	367
9.5 Analysis of Temperature Data Using a Coupled Conduction/Convection Model.....	368
9.5.1 Percolation Flux Analysis Using Qualified Temperature Data	369
9.5.2 Percolation Flux Analysis Using Non-Qualified and Qualified Temperature Data	370
9.6.3 Percolation Flux Through the Calico Hills Using Non-Qualified Data	374
9.6.4 Combined Numerical Analysis of Temperature Gradients in TSw and CHn Using Both Qualified and Non-Qualified Data	376
9.7 Concluding Remarks	376
9.8 References.....	377
<hr/>	
CHAPTER 10:	
PRELIMINARY CONCEPTUAL MODEL OF FLOW PATHWAYS BASED ON ³⁶Cl AND	
OTHER ENVIRONMENTAL ISOTOPES	
J. FAIRLEY AND E. SONNENTHAL	380
<hr/>	
10.1 Introduction	381
10.1.1 ³⁶ Cl: Measurements, Assumptions, Caveats	381
10.1.2 Unsaturated Zone (UZ) Flow Model Calibration	383
10.1.3 Changes in the UZ Flow Model Based on Environmental Isotopes	384
10.1.4 Objective of work	387
10.2 Conceptual Model Development	388
10.3 Numerical Hypothesis Testing	395
10.3.1 Approach	395
10.3.2 Methods and Results	397
10.4 Discussion of Results.....	403

Table of Contents

10.5 Locations of Fast Pathways and Predictions	407
10.6 Summary and Conclusions/Recommendations	410
10.7 References	412
<hr/>	
CHAPTER 11:	
SUBMODEL OF PERCOLATION FLUX AT THE REPOSITORY	
<i>E. SONNENTHAL, S. FINSTERLE, AND G.S. BODVARSSON</i>	416
<hr/>	
11.1 Introduction	417
11.2 Approach	418
11.3 Quality Assurance Status of Data and Software Used In This Chapter	418
11.4 Selection of a Submodel of the UZ Model	418
11.5 Geology of the Submodel Area	419
11.6 The TOUGH2 Code and Equation of State Modules	421
11.7 Evaluation of Coarse Flows From the UZ Model	422
11.8 Development of the UZ Submodel	426
11.8.1 Numerical Grid	426
11.8.2 Initial and Boundary Conditions	427
11.9 Numerical Simulations	427
11.9.1 Steady-State Liquid Fluxes, Saturations and Temperature Gradients	428
11.9.2 Comparison to UZ Model Results	435
11.9.3 Development of a 3D heterogeneous permeability field	435
11.9.4 Steady state results for heterogeneous permeability field	439
11.10 Summary	443
11.11 References	444

Table of Contents

CHAPTER 12:

SIMULATION OF COUPLED PROCESSES IN A TWO-DIMENSIONAL WEST-EAST CROSS-SECTION OF YUCCA MOUNTAIN, NEVADA

S. FINSTERLE, T. M. BANDURRAGA, C. DOUGHTY, AND G.S. BODVARSSON447

12.1 Introduction	448
12.1.1 Importance of Coupled Processes at Yucca Mountain	448
12.1.2 Purpose of Study	449
12.1.3 QA Status of Data and Software Used in this Chapter	449
12.2 Model Development	450
12.2.1 Two-Dimensional Cross-Section	450
12.2.2 Hydrostratigraphy	452
12.2.3 Initial and Boundary Conditions	455
12.3 Steady-State Conditions	456
12.3.1 Saturation	456
12.3.2 Water Potentials	460
12.3.3 Temperature	461
12.4 Gas Flow	469
12.4.1 Introduction	469
12.4.2 Gas Circulation Pattern	469
12.4.3 Barometric Pressure Response	471
12.5 Liquid Flow and Transport	472
12.5.1 Liquid Flow Rates	472
12.5.2 Fast Path	473
12.6 Summary and Concluding Remarks	475
12.7 References	477

Table of Contents

CHAPTER 13:

THERMAL LOADING STUDIES USING THE UNSATURATED ZONE MODEL

C. HAUKWA AND Y.S. WU480

13.1 Introduction	481
13.1.1 Importance of the Thermal Loading Studies	481
13.1.2 Thermal Loading and the UZ Model	481
13.1.3 Thermal Goals	482
13.1.4 Purpose of this Study	482
13.1.5 Modeling Approach.....	482
13.2 ECM simulation Results with 0.1 mm/year Infiltration	486
13.2.1 Temperatures	486
13.2.2 Saturation	490
13.2.3 Percolation Flux	493
13.3 ECM Simulation Results with 4.4 mm/year Infiltration.....	496
13.3.1 Temperature	496
13.3.2 Saturation	500
13.3.3 Percolation Flux.....	504
13.4 Dual-k Simulation Results with 4.4 mm/year Infiltration	506
13.4.1 Temperature	506
13.4.2 Saturation	511
13.4.3 Percolation Flux	517
13.5 Comparisons of Percolation Fluxes Using the Two Modeling Approaches.	520
13.5.1 Liquid Fluxes	520
13.5.2 Gas Fluxes	522
13.6 Concluding Remarks	523
13.6 References.....	525

Table of Contents

CHAPTER 14:

FRACTURE COATINGS AND FRACTURE CHARACTERISTICS WITH IMPLICATIONS FOR FLOW ALONG FAST PATHWAYS

A. SIMMONS	527
14.1 Introduction	528
14.1.1 Quality Assurance Status of Data and Software Used in This Chapter	529
14.2 Fracture Distribution and Characterization	529
14.3 Distribution and Characterization of Fracture Coatings	534
14.3.1 Stratigraphic Control	535
14.3.2 Sequence of Coatings in TSw	535
14.3.3 Calcite	536
14.4 Flux	537
14.5 Simulations of Formation of Fracture Coatings	540
14.6 Uncertainties	541
14.7 Summary and Recommendations	542
14.8 References	543

List of Figures

List of Figures

CHAPTER 1

Figure 1.1.1	A Schematic Cross Section through Yucca Mountain showing Various Conceptual Model Data and Processes.	5
Figure 1.1.2	Perched Water Elevation Data	10
Figure 1.1.3	Isopach Contour Map of the Thickness of Zeolitic Zone Above Water Table	11
Figure 1.1.4	Southeast to northwest cross section showing the conceptual idea of perched water on top of the zeolitic Calico Hills unit.	12

CHAPTER 2

Figure 2.2-1	Extended Model and Project Boundaries.	35
Figure 2.3.2-1	Core Sample Porosity and Saturations Measurements for Borehole SD-9.	41
Figure 2.3.2-2	Core Sample Capillary Pressure Measurements for Borehole SD-9.	42
Figure 2.4.1-1	Tiva Canyon Hydrogeological Unit Bottom Elevation Contour Map.	47
Figure 2.4.2-1	PTn Isopach Contour Map.	48
Figure 2.4.2-2	Yucca Mountain Tuff Isopach Map. Thickness in meters.	49
Figure 2.4.3-1	TSw Isopach Contour Map.	50
Figure 2.4.4-1	Calico Hills Formation Isopach Map.	52
Figure 2.4.5-1	Water Table Map.	53

CHAPTER 3

Figure 3.4.3-1	Liquid Saturation and Capillary Pressure for Borehole SD-7.	81
Figure 3.4.3-2	Liquid Saturation and Capillary Pressure for Borehole SD-9.	81
Figure 3.4.3-3	Liquid Saturation and Capillary Pressure for Borehole UZ-14.	82

List of Figures

Figure 3.4.3-4	Liquid Saturation Profiles for Boreholes SD-12 and UZ#16.	82
Figure 3.4.3-5	Model Layer Parameter Sensitivity.	85
Figure 3.4.3-6	Liquid saturation sensitivity coefficients with respect to matrix permeability and fracture alpha of layer tsw31 vs. Elevation for borehole SD-7. 0.1 mm/yr uniform infiltration rate inversion.	86
Figure 3.4.3-7	Normalized Standard Deviations (NSD) of Parameter Estimates for Model Layers, 0.1 mm/yr inversion.	88
Figure 3.4.4-1	Liquid Saturation and Capillary Pressure for Borehole SD-7 at Various Infiltration Rates.	90
Figure 3.4.4-2	Matrix Permeability Change for Uniform Rate Combined Column Inversions.	95
Figure 3.4.4-3	Fracture Permeability Change for Uniform Rate Combined Column Inversions.	96
Figure 3.4.4-4	Matrix van Genuchten alpha Change for Uniform Rate Combined Column Inversions.	97
Figure 3.4.4-5	Fracture van Genuchten alpha Change for Uniform Rate Combined Column Inversions.	98
Figure 3.4.4-6	Matrix van Genuchten m Change for Uniform Rate Combined Column Inversions.	99
Figure 3.4.4-7	Fracture van Genuchten m Change for Uniform Rate Combined Column Inversions.	99
Figure 3.4.4-8	Pre- and Post-Calibration Calculated Combined Column Inversion Saturations vs. Measured Data. 0.1 mm/yr case.	101
Figure 3.4.4-9	Pre- and Post-Calibration Calculated Combined Column Inversion Saturations vs. Measured Data. 5.0 mm/yr case.	101
Figure 3.4.4-10	Sensitivity of Matrix Permeability Parameters to Inversion Data at Various Uniform Infiltration Rates.	102
Figure 3.4.4-11	Sensitivity of Fracture van Genuchten alpha Parameters to Inversion Data at Various Uniform Infiltration Rates.	103
Figure 3.4.4-12	Range In Matrix Permeability Parameter Values For 0.1 mm/yr and 5 mm/yr Combined Column Inversions. Ranges are +/- one joint standard deviation.	104

List of Figures

Figure 3.5.2-1	Borehole SD-7 Calculated Saturations and Capillary Pressures From Fine Grid Column.	107
Figure 3.5.2-2	Borehole SD-9 Calculated Saturations And Capillary Pressures From Fine Grid Column.	108
Figure 3.5.2-3	Differences in Matrix Parameter Sets From SD-7 and -9 Fine-Grid Inversions.....	109
Figure 3.5.2-4	Differences in Fracture Parameter Sets From SD-7 and -9 Fine-Grid Inversions. ...	110
Figure 3.5.2-5	Normalized Conditional Standard Deviation for Model Layer Parameters.	111
Figure 3.5.3-1	Differences in Matrix Parameter Sets From Coupled Parameter And Spatially Variable Infiltration Inversions And Initial Estimate Data Set.	116
Figure 3.5.3-2	Differences in fracture parameter sets from coupled parameter and spatially variable infiltration inversions and initial estimate data set.	117
Figure 3.5.4-1	Comparison of Layer-Average Borehole Core Sample Water Potential Data and In-Situ Measurements.	119
Figure 3.5.5-1	Differences in matrix parameter sets from varying all parameters inversion and varying all parameters with different initial parameter estimates inversion.	121
Figure 3.5.5-2	Differences In Fracture Parameter Sets From Varying All Parameters Inversion And Varying All Parameters With Different Initial Parameter Estimates Inversion.	121

CHAPTER 4

Figure 4.2.1	Space discretization and geometry data in the integral finite difference method.	142
Figure 4.2.2	Idealized "double porosity" model of a fractured porous medium.	142
Figure 4.2.3	Subgridding in the method of "multiple interacting continua" (MINC).	143
Figure 4.2.4	Flow connections in the "dual permeability" model.	144
Figure 4.3.1.1	Inverse modeling flow chart.	147
Figure 4.3.2.1	True, measured, and calculated system response, definition of measurement and modeling error.	149
Figure 4.3.2.2	Confidence region, joint and conditional standard deviation	152

List of Figures

CHAPTER 5

Figure 5.3.1	1996 Site Scale model, 2-D "FY96 UZ Model" grid.....	176
Figure 5.3.2	1996 Site Scale model, 2-D "Gas Effects" grid.	177
Figure 5.3.3	Example of Grid Design in Fault Zones	180
Figure 5.3.4	East-West vertical cross-section through the 3-D model showing hydrogeological layering and offsets on the explicitly modeled faults.	181
Figure 5.4.1	Steady State Liquid Saturation distribution using the original coarse grid with an infiltration rate of 0.1 mm/year.	187
Figure 5.4.2	Steady State Capillary Pressure distribution using the original coarse grid with infiltration rate of 0.1 mm/year.	187
Figure 5.4.3	Volume-weighted percentage difference in Liquid Saturation between the coarse grid and the grid with vertical and horizontal refinement, for infiltration rate of 0.1 mm/year.	188
Figure 5.4.4	Volume-weighted percentage difference in Capillary Pressure between the coarse grid and the grid with vertical and horizontal refinement, for infiltration rate of 0.1 mm/year.	188

CHAPTER 6

Figure 6.3.1	Schematic diagram of a one-dimensional column of grid blocks	194
Figure 6.4.1	One-dimensional column extracted from the site-scale model of the unsaturated zone at Yucca Mountain, representative of conditions at well SD-7.	196
Figure 6.5.1	Steady-state liquid saturation profile for 0.1 mm/yr infiltration, using the ECM.	199
Figure 6.5.2	Steady-state liquid saturation profile for 0.1 mm/yr infiltration, using the 1-k and 5-k dual-permeability models.	200
Figure 6.5.3	Steady-state fracture flow profile for 0.1 mm/yr infiltration, using the dual-permeability models.	201
Figure 6.5.4	Steady-state liquid saturation profile for 0.1 mm/yr infiltration, using the 1-p and 5-p dual-porosity models.....	202

List of Figures

Figure 6.5.5	Liquid saturation as a function of time at the bottom of each hydrological unit and in the upper portion of the Topopah, for a one-week pulse of high infiltration, using the ECM.	206
Figure 6.5.6	Liquid saturation in the fractures as a function of time at the bottom of each hydrogeologic unit and in the upper portion of the Topopah, for a one-week pulse of high infiltration, using the 1-k model.	207
Figure 6.5.7	Liquid saturation in the fractures as a function of time at the bottom of each hydrogeologic unit and in the upper portion of the Topopah, for a one-week pulse of high infiltration, using the 5-k model.	207
Figure 6.5.8	Liquid saturation in the fractures as a function of time at the bottom of each hydrogeologic unit and in the upper portion of the Topopah, for a one-week pulse of high infiltration, using the 1-p model.	208
Figure 6.5.9	Liquid saturation in the fractures as a function of time at the bottom of each hydrogeologic unit and in the upper portion of the Topopah, for a one-week pulse of high infiltration, using the 5-p model.	208
Figure 6.5.10	Liquid saturation in the fractures as a function of time at the bottom of each hydrogeologic unit and in the upper portion of the Topopah, for a one-week pulse of high infiltration, using the fracture-only model.	209
Figure 6.5.11	Liquid saturation in the fractures as a function of time for a one-week pulse of high infiltration, using the 5-k model, and a range of areas for fracture-matrix interaction. As area decreases, liquid saturation changes in the fractures occur earlier.	210
Figure 6.5.12	Pneumatic response for the ECM and dual-permeability models at the bottom of the various hydrogeologic units.	213
Figure 6.5.13	Pneumatic response for the dual-porosity models at the bottom of the various hydrogeologic units.	213
Figure 6.5.14	Pneumatic response for the fracture-only model at the bottom of the various hydrogeologic units.	214
Figure 6.5.15	Tracer concentration as a function of time at depths corresponding to the bottom of the TCw, PTn, TSw, and CHn, for a model with no vertical variation in properties, for an infiltration rate of 0.1 mm/yr, using the ECM.	216

List of Figures

Figure 6.5.16	Tracer concentration as a function of time for a model with no vertical variation in properties for an infiltration rate of 0.1 mm/yr, using the 1-k model.	216
Figure 6.5.17	Tracer concentration as a function of time for a model with no vertical variation in properties for an infiltration rate of 0.1 mm/yr, using the 5-k model..	217
Figure 6.5.18	Tracer concentration as a function of time at depths corresponding to the bottom of the TCw, PTn, TSw, and CHn, for a model with no vertical variation in properties, for an infiltration rate of 0.1 mm/yr, using the 1-p and the 5-p models.	217
Figure 6.5.19	Tracer concentration as a function of time at depths corresponding to the bottom of the TCw, PTn, TSw, and CHn, for a model with no vertical variation in properties, for an infiltration rate of 0.1 mm/yr, using the fracture-only model.	218
Figure 6.5.20	Tracer concentration as a function of time for a model with no vertical variation in properties for an infiltration rate of 0.1 mm/yr, using the 1-k model with the source in the fracture only.	218
Figure 6.5.21	Temperature as a function of time at the bottom of each hydrogeologic unit and at the repository, for an initial thermal load of 83 kW/acre and a 0.1 mm/yr infiltration rate, obtained with the ECM.	221
Figure 6.5.22	Liquid saturation as a function of time at the bottom of each hydrogeologic unit and at the repository, for an initial thermal load of 83 kW/acre and a 0.1 mm/yr infiltration rate, obtained with the ECM.	221
Figure 6.5.23	Mass flow rate as a function of time above and below the repository, for an initial thermal load of 83 kW/acre and a 0.1 mm/yr infiltration rate, obtained with the ECM.	222
Figure 6.5.24	Temperature as a function of time at the bottom of each hydrogeologic unit and at the repository, for an initial thermal load of 83 kW/acre and a 0.1 mm/yr infiltration rate, obtained with the 1-k model.	223
Figure 6.5.25	Liquid saturation as a function of time at the bottom of each hydrogeologic unit and at the repository, for an initial thermal load of 83 kW/acre and a 0.1 mm/yr infiltration rate, obtained with the 1-k model.	224

List of Figures

Figure 6.5.26	Mass flow rate as a function of time above the repository, for an initial thermal load of 83 kW/acre and a 0.1 mm/yr infiltration rate, obtained with the 1-k model.	224
Figure 6.5.27	Mass flow rate as a function of time below the repository, for an initial thermal load of 83 kW/acre and a 0.1 mm/yr infiltration rate, obtained with the 1-k model. (Positive mass flow rate is downward.)	225
Figure 6.5.28	Temperature as a function of time at the bottom of each hydrogeologic unit and at the repository, for an initial thermal load of 83 kW/acre and a 0.1 mm/yr infiltration rate, obtained with the 1-p model.	226
Figure 6.5.29	Liquid saturation as a function of time at the bottom of each hydrogeologic unit and at the repository, for an initial thermal load of 83 kW/acre and a 0.1 mm/yr infiltration rate, obtained with the 1-p model.	226
Figure 6.5.30	Mass flow rate as a function of time above and below the repository, for an initial thermal load of 83 kW/acre and a 0.1 mm/yr infiltration rate, obtained with the 1-p model.	227

CHAPTER 7

Figure 7.3.1.1	Locations of boreholes with perched water occurrence and a plan view of the site-scale model domain, showing model boundary, computational grid, major incorporated faults, and the Exploratory Study Facility (ESF).	236
Figure 7.4.1	Perched water locations projected to a N-S cross-section their and relationships with vitric and zeolitic unit boundaries.	240
Figure 7.4.2	Contour map of the thickness of zeolites above water table and below the base of the TSw, indicating possible flow paths and lateral diversions.	241
Figure 7.5.1.1	A plan view of the site-scale model grid and the sub-model domain for perched water studies.	243
Figure 7.5.2.1	Net infiltration map (Map #1) showing infiltration rates and distributions over Yucca Mountain (Hevesi and Flint, 1995).	245
Figure 7.5.2.2	Net infiltration map (Map #2) showing infiltration rates and distributions over Yucca Mountain (Flint et al., 1996).	246
Figure 7.5.3.1	Locations and plan view of four vertical cross sections and associated boreholes.	250

List of Figures

Figure 7.5.3.2	Comparisons of the simulated and observed values for perched water in Borehole UZ-1/14; (a) saturation, (b) capillary pressure.	252
Figure 7.5.3.3	Comparisons of the simulated and observed values for perched water in Borehole NRG-7a; (a) saturation, (b) capillary pressures.	253
Figure 7.5.3.4	Comparisons of the simulated and observed values for perched water in Borehole SD-7; (a) saturation, (b) capillary pressures.	253
Figure 7.5.3.5	Comparisons of the simulated and observed values for perched water in Borehole SD-9; (a) saturation, (b) capillary pressures.	254
Figure 7.5.3.6	A plan view of saturation contours in the base of TSw showing the perched water body around UZ-1/14, SD-9 and NRG-7a.	256
Figure 7.5.3.7	A plan view of capillary pressure contours in the base of TSw showing the perched water body around UZ-1/14, SD-9 and NRG-7a.	256
Figure 7.5.3.8	Liquid saturation along the West-East section crossing borehole UZ-1/14	257
Figure 7.5.3.9	Liquid saturation along the South-North section crossing borehole UZ-1/14.	258
Figure 7.5.3.10	Liquid saturation along the West-East section crossing borehole SD-7.	259
Figure 7.5.3.11	Liquid saturation along the South-North section crossing borehole SD-7.	259
Figure 7.5.3.12	Three-dimensional saturation distributions, indicating the higher saturation zones for the perched water bodies.	260
Figure 7.5.3.13	Three-dimensional capillary pressures, indicating the lower capillary in the perched water bodies.	260
Figure 7.5.3.14	Comparison of the observed and simulated water levels for test#2 in borehole UZ-14 using a linear plot.	262
Figure 7.5.3.15	Comparison of the observed and simulated water levels for test#2 in borehole UZ-14, using a semi-log plot.	263
Figure 7.5.3.16	Comparison of the observed and simulated water levels for test#2 in borehole UZ-14 using a Horner plot.	263
Figure 7.5.3.17	Comparison of the observed and simulated water levels for test#4 in borehole UZ-14, using a linear scaled plot.	264
Figure 7.5.3.18	Comparison of the observed and simulated water levels for est#4 in borehole UZ-14, using a semi-log plot.	264

List of Figures

Figure 7.5.3.19	Comparison of the observed and simulated water levels for test#4 in borehole UZ-14, using a Horner plot.	265
-----------------	---	-----

CHAPTER 8

Figure 8.3.1	A plan view of the 3-D site-scale model domain, grid and incorporated major faults.	277
Figure 8.3.2	Temperature map at the water table for the bottom temperature boundary condition of the 3-D site-scale model.	280
Figure 8.3.3	Temperature map on the ground surface for the top temperature boundary condition of the 3-D site-scale model.	281
Figure 8.4.1	Net infiltration map (Map # 1) showing infiltration rates and distributions over the model domain of Yucca Mountain, based on Maxey-Eakin model (Hevesi and Flint, Nov., 1995).	283
Figure 8.4.2	Net infiltration map (Map # 2) showing infiltration rates and distributions over the model domain of Yucca Mountain (Flint, Hevesi and Flint, July, 1996).	284
Figure 8.6.1	Comparisons of the simulated and observed saturations and water potentials of boreholes UZ-1/14 using parameter set #4 and infiltration map #2; (a) comparisons with saturation, (b) comparisons with capillary pressure	294
Figure 8.6.2	Comparisons of the simulated and observed saturations of borehole NRG-7a using parameter set #1 and infiltration of 0.1 mm/yr; (a) comparisons with saturation, (b) capillary pressure.	295
Figure 8.6.3	Comparisons of the simulated and observed saturations and water potentials of borehole SD-7 using parameter set #4 and infiltration map #2; (a) comparisons with saturation, (b) comparisons with capillary pressure.	296
Figure 8.6.4	Comparisons of the simulated and observed saturations and water potentials of borehole SD-9 using parameter set #4 and infiltration map #2; (a) comparisons with saturation, (b) comparisons with capillary pressure.	297
Figure 8.6.5	Comparisons of the simulated and observed saturations and water potentials of borehole SD-12 using parameter set #1 and infiltration of 0.1 mm/yr; (a) comparisons with saturation, (b) comparisons with capillary pressure.	298

List of Figures

Figure 8.6.6	Comparisons of the simulated and observed saturations of borehole UZ#16 using parameter set #4 and infiltration map #2; (a) comparisons with saturation, (b) capillary pressure.	299
Figure 8.6.7	Comparisons of the simulated and observed saturations of borehole NRG-6 using parameter set #1 and infiltration of 01. mm/yr; (a) comparisons with saturation, (b) capillary pressure.	300
Figure 8.7.1	Location and plan view of four vertical cross sections and associated boreholes. ...	301
Figure 8.7.2	Velocity fields and liquid saturations along the West-East cross section crossing UZ-1/14, simulated using parameter set #1 and infiltration of 0.1 mm/yr.	302
Figure 8.7.3	Velocity fields and liquid saturations along the West-East cross section crossing UZ-1/14, simulated using parameter set #2 and infiltration of 0.1 mm/yr.	302
Figure 8.7.4	Velocity fields and liquid saturations along the West-East cross section crossing UZ-1/14, simulated using parameter set #3 and infiltration map #1.	303
Figure 8.7.5	Velocity fields and liquid saturations along the West-East cross section crossing UZ-1/14, simulated using parameter set #4 and infiltration map #2.	303
Figure 8.7.6	Velocity fields and liquid saturations along the South-North cross section crossing UZ-1/14, simulated using parameter set #1 and infiltration of 0.1 mm/yr.	305
Figure 8.7.7	Velocity fields and liquid saturations along the South-North cross section crossing UZ-1/14, simulated using parameter set #2 and infiltration of 0.1 mm/yr.	305
Figure 8.7.8	Velocity fields and liquid saturations along the South-North cross section crossing UZ-1/14, simulated using parameter set #3 and infiltration map #1.	306
Figure 8.7.9	Velocity fields and liquid saturations along the South-North cross section crossing UZ-1/14, simulated using parameter set #4 and infiltration map #2.	306
Figure 8.7.10	Velocity fields and liquid saturations along the West-East cross section crossing SD-7, simulated using parameter set #1 and infiltration of 0.1 mm/yr.	307

List of Figures

Figure 8.7.11	Velocity fields and liquid saturations along the West-East cross section crossing SD-7, simulated using parameter set #2 and infiltration of 0.1 mm/yr.	308
Figure 8.7.12	Velocity fields and liquid saturations along the West-East cross section crossing SD-7, simulated using parameter set #3 and infiltration map #1.	308
Figure 8.7.13	Velocity fields and liquid saturations along the West-East cross section crossing SD-7, simulated using parameter set #4 and infiltration map #2.	309
Figure 8.7.14	Velocity fields and liquid saturations along the South-North cross section crossing SD-7, simulated using parameter set #1 and infiltration of 0.1 mm/yr.	310
Figure 8.7.15	Velocity fields and liquid saturations along the South-North cross section crossing SD-7, simulated using parameter set #2 and infiltration of 0.1 mm/yr.	310
Figure 8.7.16	Velocity fields and liquid saturations along the South-North cross section crossing SD-7, simulated using parameter set #3 and infiltration map #1.	311
Figure 8.7.17	Velocity fields and liquid saturations along the South-North cross section crossing SD-7, simulated using parameter set #4 and infiltration map #2.	311
Figure 8.7.18	Saturations at the repository horizon and below, simulated using parameter set #1 and infiltration of 0.1 mm/yr.	314
Figure 8.7.19	Saturations at the repository horizon and below, simulated using parameter set #4 and infiltration map #2.	314
Figure 8.7.20	Saturations at the repository horizon and below, simulated using parameter set #4 and infiltration map #2.	315
Figure 8.7.21	Velocity components in the west-east direction at the middle of the PTn, and below, simulated using parameter set #1 and infiltration of 0.1 mm/yr.	316
Figure 8.7.22	Velocity components in the south-north direction at the middle of the PTn, and below, simulated using parameter set #1 and infiltration of 0.1 mm/yr.	317

List of Figures

Figure 8.7.23	Velocity components in the vertical direction at the middle of the PTn, and below, simulated using parameter set #1 and infiltration of 0.1 mm/yr.	318
Figure 8.7.24	Velocity components in the west-east direction at the middle of the PTn, and below, simulated using parameter set #4 and infiltration map #2.	319
Figure 8.7.25	Velocity components in the south-north direction at the middle of the PTn, and below, simulated using parameter set #4 and infiltration map #2.	319
Figure 8.7.26	Velocity components in the vertical direction at the middle of the PTn, and below, simulated using parameter set #4 and infiltration map #2.	320
Figure 8.7.27	3-D temperature distributions in the unsaturated zone of Yucca Mountain, simulated using parameter set #4 and infiltration map #2.	321
Figure 8.7.28	Vertical heat flow map at repository horizon of the unsaturated zone of Yucca Mountain, simulated using parameter set #4 and infiltration map #2.	322
Figure 8.8.1	Moisture movement and distributions along the West-East cross section crossing SD-7, Solitario Canyon, Ghost Dance and Dune Wash faults, simulated using fault #1 properties, parameter set #1 and infiltration of 0.1 mm/yr.	323
Figure 8.8.2	Moisture movement and distributions along the West-East cross section crossing SD-7, Solitario Canyon, Ghost Dance and Dune Wash faults, simulated using fault #1 properties, parameter set #2 and infiltration of 0.1 mm/yr.	324
Figure 8.8.3	Moisture movement and distributions along the West-East cross section crossing SD-7, Solitario Canyon, Ghost Dance and Dune Wash faults, simulated using fault #1 properties, parameter set #3 and infiltration map #1.	324
Figure 8.8.4	Moisture movement and distributions along the West-East cross section crossing SD-7, Solitario Canyon, Ghost Dance and Dune Wash faults, simulated using fault #1 properties, parameter set #4 and infiltration map #2.	325

List of Figures

Figure 8.8.5	Moisture movement and distributions along the West-East cross section crossing SD-7, Solitario Canyon, Ghost Dance and Dune Wash faults, simulated using fault #2 properties, parameter set #1 and 0.1 mm/yr infiltration.	326
Figure 8.8.6	Moisture movement and distributions along the West-East cross section crossing SD-7, Solitario Canyon, Ghost Dance and Dune Wash faults, simulated using fault #3 properties, parameter set #4 and infiltration map #2.	327
Figure 8.8.7	Moisture movement and distributions along the West-East cross section crossing UZ-1/14 and Solitario Canyon fault, simulated using fault #1 properties, parameter set #1 and infiltration of 0.1 mm/yr.	328
Figure 8.8.8	Moisture movement and distributions along the West-East cross section crossing UZ-1/14 and Solitario Canyon fault, simulated using fault #2 properties, parameter set #1 and infiltration of 0.1 mm/yr.	328
Figure 8.8.9	Moisture movement and distributions along the West-East cross section crossing UZ-1/14 and Solitario Canyon fault, simulated using fault #1 properties, parameter set #4 and infiltration map #2.	329
Figure 8.8.10	Moisture movement and distributions along the West-East cross section crossing UZ-1/14 and Solitario Canyon fault, simulated using fault #3 properties, parameter set #4 and infiltration map #2.	329
Figure 8.9.1	Comparisons of the observed and simulated saturations and capillary pressures using dual-permeability and ECM approaches at borehole SD-7 with parameter set #4 and infiltration map #2; (a) matrix saturation, (b) matrix capillary pressure.	332
Figure 8.9.2	Comparisons of the observed and simulated fracture saturations using dual-permeability and ECM approaches at borehole SD-7 with parameter set #4 and infiltration map #2.	333
Figure 8.9.3	Matrix liquid saturations and velocity fields after 100 years along the West-East cross section crossing UZ-1/14, simulated using a dual-permeability approach and high-pulse infiltration rate.	334
Figure 8.9.4	Fracture liquid saturations and velocity fields in 100 years along the West-East cross section crossing UZ-1/14, simulated using a dual-permeability approach and high-pulse infiltration rate.	334

List of Figures

Figure 8.9.5	Matrix liquid saturations and velocity fields in 1,000 years along the West-East cross section crossing UZ-1/14, simulated using a dual-permeability approach and high-pulse infiltration rate.	335
Figure 8.9.6	Fracture liquid saturations and velocity fields in 1,000 years along the West-East cross section crossing UZ-1/14, simulated using a dual-permeability approach and high-pulse infiltration rate.	336
Figure 8.9.7	Matrix liquid saturations and velocity fields in 30,000 years along the West-East cross section crossing UZ-1/14, simulated using a dual-permeability approach and high-pulse infiltration rate.	336
Figure 8.9.8	Fracture liquid saturations and velocity fields at 30,000 years along the West-East cross section crossing UZ-1/14, simulated using a dual-permeability approach and high-pulse infiltration rate.	337
Figure 8.9.9	Matrix the saturations and velocity fields in 100,000 years along the West-East cross section crossing UZ-1/14, simulated using a dual-permeability approach and high-pulse infiltration rate.	337
Figure 8.9.10	Fracture liquid saturations and velocity fields in 100,000 years along the West-East cross section crossing UZ-1/14, simulated using a dual-permeability approach and high-pulse infiltration rate.	338
Figure 8.10.1	Percolation fluxes at the repository horizon, simulated using the ECM model, parameter set #1 and uniform infiltration rate of 0.1 mm/yr.	339
Figure 8.10.2	Percolation fluxes at the repository horizon, simulated using the ECM model, parameter set #2 and uniform infiltration rate of 0.1 mm/yr.	340
Figure 8.10.3	Percolation fluxes at the repository horizon, simulated using the ECM model, parameter set #3 and infiltration map #1.	340
Figure 8.10.4	Percolation fluxes at the repository horizon, simulated using the ECM model, parameter set #4 and infiltration map #2.	341
Figure 8.10.5	Fracture percolation fluxes at the repository horizon, simulated using the dual-permeability model, parameter set #4 and infiltration map #2.	341
Figure 8.10.6	Matrix percolation fluxes at the repository horizon, simulated using the dual-permeability model, parameter set #4 and infiltration map #2.	342
Figure 8.10.7	Recharge map at the water table, simulated using the ECM model, parameter set #1 and uniform infiltration rate of 0.1 mm/yr.	344
Figure 8.10.8	Recharge map at the water table, simulated using the ECM model, parameter set #2 and uniform infiltration rate of 0.1 mm/yr.	345

List of Figures

Figure 8.10.9	Recharge map at the water table, simulated using the ECM model, parameter set #3 and infiltration map #1.	345
Figure 8.10.10	Recharge map at the water table, simulated using the ECM model, parameter set #4 and infiltration map #2.	346
Figure 8.10.11	Recharge map at the water table, simulated using the dual-permeability model, parameter set #4 and infiltration map #2.	346
Figure 8.10.12	Recharge map at the water table, simulated using the dual-permeability model, parameter set #4 and infiltration map #2.	347

CHAPTER 9

Figure 9.3.1	Map of borehole locations used for the conduction study and the study area of the site-scale model.	360
Figure 9.3.2	Observed temperature profiles for UE-25: a#6, a#7 and b#.	361
Figure 9.3.3	Observed temperature profiles for UE-25: a#1, a#4 and a#5.	361
Figure 9.3.4	Observed temperature profiles for G-series boreholes, USW G-1, G-2, G-3 and G-4.	362
Figure 9.3.5	Observed temperature profiles for H-series boreholes, USW H-1, H-2, H-3 and H-4.	362
Figure 9.3.6	Observed temperature profiles for USW UZ-1, WT-1, WT-2, WT#4 and WT#6.	363
Figure 9.3.7	Observed temperature profiles for USW WT-7, WT-10, WT#16, WT#17 and WT#18.	363
Figure 9.3.8	Observed temperature profiles for UZ-4, UZ-5, UZ-7a, SD-12, NRG-6 and NRG-7a.	364
Figure 9.3.9	Heat flow distribution in the unsaturated zone (mW/m^2) taken from Sass et al. (1988).	365
Figure 9.4.1	Comparison between measured temperature data for well H-3 (Sass et al., 1988) and various ITOUGH2 optimized profiles.	367
Figure 9.4.2	Comparison between measured temperature data for well H-5 (Sass et al., 1988) and various ITOUGH2 optimized profiles.	367
Figure 9.5.1	Locations of boreholes used in the coupled convection/conduction analysis superimposed on an elevation contour map.	371

List of Figures

Figure 9.5.2	Temperature gradient contour map for the Topopah Springs Unit based on qualified and non-qualified temperature data for the boreholes shown.	372
Figure 9.5.3	Spatial distribution of percolation flux at the repository horizon using Flint et al. (1996) infiltration map.	373
Figure 9.5.4	Approximate temperature gradient contour map for the Calico Hills Unit based on qualified and non-qualified temperature data for the boreholes shown.	375

CHAPTER 10

Figure 10.1.3.1.1	Cross-section of Yucca Mountain between Ghost Dance fault and Bow Ridge fault showing location of perched water at SD-7, location of bomb-pulse ^{36}Cl in neutron hole UZN-55 and location of bomb-pulse tritium in UZ-16.	385
Figure 10.1.3.2.1	Map of UZ model showing model grid, trace of major faults, trace of ESF and boreholes where perched water was detected.	386
Figure 10.3.1a	Hypothesis "A"	391
Figure 10.3.1b	Hypothesis "B"	392
Figure 10.3.1c	Hypothesis "C"	393
Figure 10.3.1.1	Representation of grid for schematic fast pathways model.	396
Figure 10.3.1.2	Character curves for two simulated fault zones.	397
Figure 10.3.2.1	Normalized concentrations of tracer as a function of depth below landsurface.	399
Figure 10.3.2.2	Normalized concentrations of two different effective fault apertures: 0.5mm and 1.0mm. Infiltration pulses shown are 10cm/wk.	400
Figure 10.3.2.3	Normalized concentrations of tracer in a simulated fault zone as a function of depth below landsurface.	401
Figure 10.3.2.4	Effect of PTn thickness on arrival concentrations of tracer at depth.	402
Figure 10.3.2.5	Effect of PTn thickness on arrival concentrations of tracer as a function of depth, for a pulse size of 50cm/wk, and an effective fault aperture of 1.0mm.	402
Figure 10.4.1	Map of near-surface infiltration, showing the Exploratory Studies Facility.	404

List of Figures

Figure 10.4.2	Width of watershed basin needed to generate an infiltration pulse.	404
Figure 10.5.1	Map of alluvial thickness at the Yucca Mountain site, showing the Exploratory Studies Facility and major faults.	409
<hr/> CHAPTER 11 <hr/>		
Figure 11.4.1	Map view of submodel.	419
Figure 11.5.1	E-W cross-section of Yucca Mountain showing hydrogeological units and major faults.	420
Figure 11.7.1	Liquid flux vectors from UZ model simulation in area around submodel domain.	423
Figure 11.7.2	Renormalized liquid flux vectors for TSw, PTn, and TCw units from UZ model simulation in area around submodel domain.	424
Figure 11.7.3	The vertical component of the fluid flux from element 185 in the UZ model normalized to the 0.1 mm/yr infiltration flux (a) and the magnitude of the flux (b).	425
Figure 11.8.1	Plan view of submodel grid showing inner rectangular mesh and coarse outer mesh.	426
Figure 11.9.1	Infiltration rates at UZ model grid nodes, as derived from Flint et al., (1996).	428
Figure 11.9.2	Steady-state fluid flux vectors for an infiltration rate of 0.1mm/yr.	429
Figure 11.9.3	Flux vectors for the upper TSw layer to the bottom of the TCw unit (partial layer on east side).	430
Figure 11.9.4	Contour map of the flux vector magnitudes for layer (TSw34-TSw33) at approximately the 1094 meter level, for an infiltration rate of 0.1 mm/yr.	431
Figure 11.9.5	Contour map of liquid saturations for layer (TSw34-TSw33) at approximately the 1094 meter level, for an infiltration rate of 0.1 mm/yr.	431
Figure 11.9.6	Contour map of the flux vector magnitudes for layer (TSw34-TSw33) at approximately the 1094 meter level, for an infiltration rate of 5.0 mm/yr.	432
Figure 11.9.7	Contour map of liquid saturations for layer (TSw34-TSw33) at approximately the 1094 meter level, for an infiltration rate of 5.0 mm/yr.	433
Figure 11.9.8	Steady-state temperature profiles from center of submodel domain for infiltration rates of 0.1 and 5.0 mm/yr.	434

List of Figures

Figure 11.9.9	Permeability contours for an E-W cross-section through center of submodel domain.	438
Figure 11.9.10	Permeability contours for the TSw34-TSw33 layer (approximately 1094m elevation), near the top of the repository horizon.	438
Figure 11.9.11	Contour map of fluid flux magnitudes at the TSw33-TSw-34 layer (1094m), for an infiltration rate of 0.1 mm/yr.	440
Figure 11.9.12	Contour map of liquid saturations at the TSw33-TSw-34 layer (1094m), for an infiltration rate of 0.1 mm/yr.	440
Figure 11.9.13	Flux vectors for the base of the TCw, the PTn and uppermost two layers of the TSw, at an infiltration rate of 5.0 mm/yr.	441
Figure 11.9.14	Contour map of fluid flux magnitudes at the TSW33-TSW-34 layer (1094m), for an infiltration rate of 5.0 mm/yr.	442
Figure 11.9.15	Contour map of liquid saturations at the TSW33-TSW-34 layer (1094m), for an infiltration rate of 5.0 mm/yr.	442

CHAPTER 12

Figure 12.2.1.1	Grid of the west-east cross-section along Nevada Coordinates N 231800.	451
Figure 12.2.2.1	Matrix permeabilities.	452
Figure 12.2.2.2	Fracture permeabilities.	453
Figure 12.2.2.3	Matrix a-parameters of the van Genuchten model.	453
Figure 12.2.2.4	Fracture a-parameters of the van Genuchten model	454
Figure 12.2.2.5	Matrix porosities.	454
Figure 12.2.3.1	Infiltration rates applied at the surface of the model, interpolated from infiltration map provided by A. Flint, USGS.	456
Figure 12.3.1.1	Simulated saturation distribution of matrix continuum.	457
Figure 12.3.1.2	Simulated saturation distribution of fracture continuum.	457
Figure 12.3.1.3	Comparison between calculated and measured saturation profile in borehole SD-7. Data from L. Flint, USGS.	458
Figure 12.3.1.4	Comparison between calculated and measured saturation profile in borehole UZ#16. Data from L. Flint, USGS.	459

List of Figures

Figure 12.3.1.5	Comparison between calculated and measured saturation profile in borehole UZ-6s. Data from C. Loskot, USGS.	459
Figure 12.3.2.1	Modeled water potential distribution.	460
Figure 12.3.2.2	Comparison between calculated and observed water potentials in borehole SD-7. Data from L. Flint, USGS.	460
Figure 12.3.3.1	Simulated temperature distribution.	462
Figure 12.3.3.2	Vertical heat flux.	462
Figure 12.3.3.3	Calculated temperature and temperature gradient in Topopah Spring along the profile.	465
Figure 12.3.3.4	Calculated percolation flux as a function of temperature gradient.	466
Figure 12.3.3.5	Impact of faults on temperature gradient and percolation flux.	466
Figure 12.3.3.6	Infiltration rate estimated from simulated temperature gradient data, compared to actually prescribed infiltration rate.	467
Figure 12.3.3.7	Comparison between calculated and measured temperature profiles in borehole UZ-7a. Data from Rousseau, USGS.	468
Figure 12.3.3.8	Comparison between calculated and measured temperature profiles in borehole H-3. Data from Sass, USGS.	468
Figure 12.4.2.1	Calculated liquid saturation in fracture continuum and gas particle tracks.	470
Figure 12.4.3.1	Simulated and observed pneumatic response to barometric pressure fluctuations in SD-7.	471
Figure 12.5.1.1	Total liquid saturation and liquid flow vectors.	473
Figure 12.5.1.2	Vertical (contours) and horizontal (vectors) flow components.	473
Figure 12.5.2.1	Simulated change of liquid saturation 50 years after release of infiltration pulse.	474
Figure 12.5.2.2	Simulated liquid saturation as function of time in fracture continuum, near borehole SD-7.	475

List of Figures

CHAPTER 13

Figure 13.1.1	Areal grid of the 3-D UZ model showing location of N-S cross-section, boreholes.	483
Figure 13.1.2	2-D UZ North-South Cross section A-A', showing model grid layers and hydrogeological units used.	484
Figure 13.1.3	Comparisons between the observed and simulated saturation for borehole UZ-14, using the 2-D section, the USGS measured values, and infiltration rate of 0.1 mm/year.	485
Figure 13.2.1	2-D UZ cross-section model.	487
Figure 13.2.2	Temperature distribution after 1000 years thermal loading.	488
Figure 13.2.3	Vertical temperature profiles through the center of the repository block during 1,000 years of thermal loading.	488
Figure 13.2.4	Temperature at various depths at the center of the repository during 100,000 years of thermal loading.	489
Figure 13.2.5	Temperature in the repository horizon during thermal loading	489
Figure 13.2.6	Temperature at the land surface during thermal loading	490
Figure 13.2.7	Ambient liquid saturation in the matrix and liquid flux, infiltration = 0.1 mm/year.	491
Figure 13.2.8	Liquid Saturation after 1000 years thermal loading APD = 83 kW/acre, infiltration = 0.1 mm/year.	492
Figure 13.2.9	Liquid saturation at various depths in the center of the repository block during 100,000 years of thermal loading.	492
Figure 13.2.10	Vertical saturation profiles through the center of the repository block during 100,000 years of thermal loading.	493
Figure 13.2.11	Liquid saturation in the repository horizon during thermal loading, APD 83 kW/acre, infiltration = 0.1 mm/year.	493
Figure 13.2.12	Gas flux profiles in the repository horizon after 1000 years emplacement.	494
Figure 13.2.13	Liquid Flux crossing the top boundary of the repository.	495
Figure 13.2.14	Liquid Flux crossing the bottom boundary of the repository'	495

List of Figures

Figure 13.3.1	Temperature distribution after 1000 years thermal loading.	497
Figure 13.3.2	Temperature distribution after 1000 years thermal loading.	497
Figure 13.3.3	Vertical temperature profiles through the center of the repository block during 10,000 years of thermal loading.	498
Figure 13.3.4	Temperature at various depths at the center of the repository during 10,000 years of thermal loading.	498
Figure 13.3.5	Temperature in the repository horizon during thermal loading.	499
Figure 13.3.6	Temperature at the land surface during thermal loading.	499
Figure 13.3.7	Matrix continuum ambient liquid saturation	501
Figure 13.3.8	Fracture continuum ambient liquid saturation; vectors show liquid flu.	501
Figure 13.3.9	Matrix continuum liquid saturation after 1000 years thermal loading.	502
Figure 13.3.10	Fracture continuum liquid saturation after 1000 years thermal loading.	502
Figure 13.3.11	Liquid saturation at various depths in the center of the repository block during 10,000 years of thermal loading.	503
Figure 13.3.12	Vertical saturation profiles through the center of the repository block during 10,000 years of thermal loading.	503
Figure 13.3.13	Liquid saturation in the repository horizon during thermal loading.	504
Figure 13.3.14	Liquid Flux crossing the top boundary of the repository	505
Figure 13.3.15	Liquid Flux crossing the bottom boundary of the repository.	505
Figure 13.4.1	Temperature distribution after 500 years thermal loading; Dual-k, APD = 83 kW/acre, infiltration = 4.4 mm/year.	507
Figure 13.4.2	Temperature distribution after 500 years thermal loading; Dual-k, APD = 83 kW/acre, infiltration = 4.4 mm/year.	597
Figure 13.4.3	Temperature distribution after 1000 years thermal loading; Dual-k, APD = 83 kW/acre, infiltration = 4.4 mm/year.	508
Figure 13.4.4	Temperature distribution after 1000 years thermal loading; Dual-k, APD = 83 kW/acre, infiltration = 4.4 mm/year.	508

List of Figures

Figure 13.4.5	Vertical temperature profiles through the center of the repository block during 25,000 years of thermal loading; Dual-k, APD = 83 kW/acre, infiltration = 4.4 mm/year.	509
Figure 13.4.6	Temperature at various depths at the center of the repository during 25,000 years of thermal loading; Dual-k, APD = 83 kW/acre, infiltration = 4.4 mm/year.	509
Figure 13.4.7	Temperature in the repository horizon during thermal loading; Dual-k, APD 83 kW/acre, infiltration = 4.4 mm/year.	510
Figure 13.4.8	Temperature at the land surface during thermal loading; Dual-k, APD 83 kW/acre, infiltration = 4.4 mm/year.	510
Figure 13.4.9	Matrix continuum ambient liquid saturation; Dual-k, APD 83 kW/acre, infiltration = 4.4 mm/year.	512
Figure 13.4.10	Fracture continuum ambient liquid saturation; vectors show liquid flux; Dual-k, APD 83 kW/acre, infiltration = 4.4 mm/year.	512
Figure 13.4.11	Matrix continuum liquid saturation after 500 years thermal loading Dual-k, APD = 83 kW/acre, infiltration = 4.4 mm/year.	513
Figure 13.4.12	Matrix continuum liquid saturation after 1000 years thermal loading Dual-k, APD = 83 kW/acre, infiltration = 4.4 mm/year.	513
Figure 13.4.13	Fracture continuum liquid saturation after 500 years thermal loading Dual-k, APD = 83 kW/acre, infiltration = 4.4 mm/year.	514
Figure 13.4.14	Fracture continuum liquid saturation after 1000 years thermal loading Dual-k, APD = 83 kW/acre, infiltration = 4.4 mm/year.	514
Figure 13.4.15a	Matrix vertical saturation profiles through the center of the repository block during 25,000 years of thermal loading; Dual-k, APD = 83 kW/acre, infiltration = 0.1 mm/year.	515
Figure 13.4.15b	Fracture vertical saturation profiles through the center of the repository block during 25,000 years of thermal loading; Dual-k, APD = 83 kW/acre, infiltration = 0.1 mm/year	515
Figure 13.4.16	Matrix Liquid saturation at various depths in the center of the repository block during 10,000 years of thermal loading; Dual-k, APD = 83 kW/acre, infiltration = 4.4 mm/year.	516
Figure 13.4.17	Fracture Liquid saturation at various depths in the center of the repository block during 10,000 years of thermal loading; Dual-k, APD = 83 kW/acre, infiltration = 4.4 mm/year.	516

List of Figures

Figure 13.4.18	Matrix Liquid saturation in the repository horizon during thermal loading; Dual-k, APD 83 kW/acre, infiltration = 4.4 mm/year.	517
Figure 13.4.19	Fracture Liquid saturation in the repository horizon during thermal loading; Dual-k, APD 83 kW/acre, infiltration = 4.4 mm/year.....	517
Figure 13.4.20	Matrix liquid flux crossing the top boundary of the repository; Dual-k, APD = 83 kW/acre, Infiltration 4.4 mm/year.	518
Figure 13.4.21	Matrix liquid flux crossing the bottom boundary of the repository; Dual-k, APD = 83 kW/acre, Infiltration 4.4 mm/year.	519
Figure 13.4.22	Fracture liquid flux crossing the top boundary of the repository; Dual-k, APD = 83 kW/acre, Infiltration 4.4 mm/year.....	519
Figure 13.4.23	Fracture liquid flux crossing the bottom boundary of the repository; Dual-k, APD = 83 kW/acre, Infiltration 4.4 mm/year.	520
Figure 13.5.1	Matrix liquid flux crossing the top and bottom boundary of the repository; for different infiltration rates; ECM and Dual-k, APD = 83 kW/acre.	521
Figure 13.5.2	Matrix liquid flux crossing the top and bottom boundary at the center of the repository; for different infiltration rates; ECM and Dual-k, APD = 83 kW/acre.	521
Figure 13.5.3	Matrix and Fracture gas flux crossing the top and bottom boundary of the repository; for different infiltration rates; ECM and Dual-k, APD = 83 kW/acre.....	522
Figure 13.5.4	Matrix and Fracture gas flux crossing the top and bottom boundary at the center of the repository; for different infiltration rates; ECM and Dual-k, APD = 83 kW/acre.	523

List of Figures

CHAPTER 14

- Figure 14.3.1 Location map showing Yucca Mountain, generalized lithologic units, and drillholes mentioned in this report from which core was analyzed by Los Alamos National Laboratory (modified from Carlos et al., 1995a).534
- Figure 14.4.1 Schematic of two conceptual models of percolation flux developed by U.S. Geological Survey and based on mineral coating apparent ages (from Peterman and Paces, 1996). t = relative time of deposition of layers. a) episodic/instantaneous model; b) continuous deposition model.539

List of Tables

CHAPTER 2

Table 2.2-1	Relationship between Model Hydrogeological Units and Geological Formations	37
-------------	--	----

CHAPTER 3

Table 3.1.5-1	Data and Numerical Uncertainties	65
Table 3.2.1-1	Saturation and Water Potential Borehole Data from USGS.	66
Table 3.2.2-1	TSPA Unit Designation and Correlation with Geologic Formations	70
Table 3.2.2-2	Matrix Hydrogeologic Parameter Comparison	71
Table 3.2.2-3	Fracture Permeability Estimates	73
Table 3.4.3-1	0.1 mm/yr Rate Residual Standard Deviation (RSD) and Bias Summary	85
Table 3.4.4-1	Residual Standard Deviation (RSD) and Bias Summary	89
Table 3.4.4-2	Summary of Calibrated Uniform Rate Model Parameters	91
Table 3.5.1-1	Spatially Variable Infiltration Rates (mm/yr)	105
Table 3.5.1-2	Residual Standard Deviation(RSD) and Bias Summary for Spatially Variable Infiltration Rates	106
Table 3.5.2-1	Fine Grid Column Residual Standard Deviation (RSD) and Bias Summary	109
Table 3.5.3-1	Sensitivity Study Parameter Sets	112
Table 3.5.4-1	Residual Standard Deviation (RSD) and Bias Summary	120

CHAPTER 4

Table 4.3.1.1	Stepwise procedure of parameter estimation by inverse modeling	146
Table 4.3.2.1	Levenberg-Marquardt algorithm	150

List of Tables

Table 4.4.1	Coefficients of multiple linear regressions relating thermal conductivity.	154
Table 4.6.1	Options for different weighting schemes in TOUGH2.	161
<hr/> CHAPTER 5 <hr/>		
Table 4.7.1	Summary of EOS1G	164
<hr/> CHAPTER 6 <hr/>		
Table 6.3.1	Types of numerical formulations for fracture-matrix flow.	195
Table 6.5.1	Fracture-fracture and fracture-matrix characteristic times*	204
Table 6.5.2	Times at which saturation increases at the bottom of the Topopah Springs and at the bottom of the Calico Hills for a one-week high-infiltration-rate pulse	205
Table 6.5.3	Gas flow diffusion time.	212
Table 6.5.4	Times at which tracer appears at depths corresponding to the bottom of the Topopah Springs and the bottom of the Calico Hills, for uniform infiltration of 0.1 mm/yr.	219
Table 6.6.1	Summary of problems considered.	228
<hr/> CHAPTER 7 <hr/>		
Table 7.3.1	Borehole location and perched water occurrence	235
Table 7.5.2.1	The rock properties of matrix and fractures for perched water studies.	247
Table 7.5.3.1	The calibrated rock matrix properties for perched water studies in the vicinity of UZ-1/14, SD-9 and NRG-7a.	251
Table 7.5.3.2	The calibrated rock matrix properties for perched water studies in the vicinity of SD-7.	252
<hr/> CHAPTER 8 <hr/>		
Table 8.2.1	Saturation and Capillary pressure Borehole Data from USGS	275
Table 8.5.1	The rock properties, parameter set #1, of matrix and fractures used in the model calibration and sensitivity studies.	286

List of Tables

Table 8.5.2	The rock properties, parameter set #2, of matrix and fractures used in the model calibration and sensitivity studies.	287
Table 8.5.3	The rock properties, parameter set #3, of matrix and fractures used in the model calibration and sensitivity studies.	288
Table 8.5.4	The rock properties, parameter set #4, of matrix and fractures used in the model calibration and sensitivity studies.	289
Table 8.5.5	The corresponding relations of rock names, geological and hydrogeological units, formation and model grid layers used in the site-scale model.	290
Table 8.5.6	The rock properties for fault #1 used in the model calibration and sensitivity studies.	292
Table 8.5.7	The rock properties for fault #2 used in the model calibration and sensitivity studies.	292
Table 8.5.8	The rock properties for fault #3 used in the model calibration and sensitivity studies.	292
Table 8.9.1	The fracture porosity, aperture and spacing data used for the dual-permeability simulations (Wilson et al., 1994).	331

CHAPTER 9

Table 9.2.1	Qualified temperature data and corresponding data tracking numbers.	357
Table 9.3.1	Location, elevation, and completion information for the selected boreholes.	359

CHAPTER 11

Table 11.5.1	Typical Thicknesses and Permeabilities of Hydrogeological Units in Submodel	421
Table 11.9.1	Steady-State Conditions at Repository Horizon For Differing Infiltration Rates	434
Table 11.9.2	Comparison of UZ model and Submodel at the Repository Horizon (0.1 mm/yr infiltration rate)	435
Table 11.9.3	Spatial Parameters Used in Simulated Annealing	437

List of Tables

CHAPTER 12

Table 12.1.2.1	Summary of Key Processes and Affected Data	449
Table 12.1.3.1	QA Status of Data Used in this Chapter	450

DEVELOPMENT OF THE UNSATURATED ZONE MODEL IN FISCAL YEAR 1996

G.S. Bodvarsson, T.M. Bandurraga, and Y.S. Wu

August 1996

1.0 Introduction

The 3-dimensional unsaturated zone model (UZ model) of Yucca Mountain is being developed by Lawrence Berkeley National Laboratory (LBNL) in collaboration with the U. S. Geological Survey (USGS). The model has evolved from crude 1-dimensional and 2-dimensional models without much geological or hydrological realism to a fully coupled three-dimensional model incorporating known geological and hydrological complexities.

The model development started with the work of Rulon et al. (1986). They used two-dimensional cross-sectional models to investigate various important flow processes at Yucca Mountain including lateral flow within the Paintbrush unit and effects of fracture and matrix flow. This work was followed by a number of studies of processes on a more basic level than site-scale coupled processes. In the early 1990's Wittwer and coworkers (1992; 1995) started the development of a complex three-dimensional model that incorporated many geological and hydrological complexities such as geological layering, degree of welding, fault offsets, differing geological layer matrix and fracture properties, and others. This work resulted in a report that addressed many processes and hydrological issues, and showed complex moisture flow patterns resulting from the geological and hydrological flow patterns considered. Ahlers et al. (1995a,b) continued the development of the Wittwer et al. UZ model with increased numerical and spatial resolution. Their studies considered several processes such as gas pressures and flow, temperature and heat flow analyses, and rock property evaluation through inverse modeling.

Various other project participants have also developed models that have enhanced the understanding of single- and coupled flow and transport processes within the unsaturated zone. Wang and Narasimhan (1987) showed that the degree of lateral flow depends strongly on assumed hydrological parameters of vertical fault zones, especially the characteristic curves. Other work by Wang and Narasimhan (1985) suggested that the effect of infiltration pulses at the surface is dampened by the underlying tuff units. Their results showed that the welded tuff unit of the potential repository horizon exhibited only small changes in saturations, pressures, and potentials from steady-state values in response to the transient pulses.

One of the first three-dimensional models was developed by Rockhold et al. (1990), who studied the unsaturated zone in the immediate vicinity of the potential repository and found considerable lateral flow due to the complex stratigra-

phy and perched water. The various cases considered indicated mostly fracture-dominated flow in the shallow welded units (Tiva Canyon), but matrix-dominated flow elsewhere.

Concurrent modeling work by the USGS includes studies by Flint et al. (1993) to predict saturation and water potential profiles in borehole UZ#16. Kwicklis et al. (1994) performed additional studies of UZ flow beneath Pagany Wash. Moyer et al. (1995) presented the results of simulation by L. Flint of the USGS studying lateral diversion. The evaluation showed that the PTn sublayers could cause lateral diversion of infiltrating moisture which was related to the variations in hydrogeological properties between adjacent sublayers and sub-layer thicknesses.

Work by other project participants includes Arnold et al. (1995), who used 2-D cross-section models to evaluate the travel time of fluid from the proposed repository level to the water table. Ho (1994) evaluated flow into a welded tuff matrix material from a saturated vertical fracture. Robinson et al. (1995) presented a report containing the results of transport modeling for various radioactive isotopes along with sensitivity analyses using various scenarios.

The continued development of the UZ model builds on the analysis and results of the above referenced work and many other studies. The primary objectives of the UZ model are as follows:

1. To develop a model that represents all of the major flow processes, including moisture, gas, and heat, along with features and events that are or will be occurring in the unsaturated zone under ambient and thermally perturbed conditions for the next 100,000 years.
2. To evaluate current and future spatial and temporal variations in percolation flux at the repository horizon and other elevations, and the components of fracture/fault versus matrix flow.
3. To evaluate impacts and effects of important hydrological features such as major faults, perched water, lateral flow barriers, and moisture, gas or heat flow conduits.
4. To evaluate various conceptual and numerical scenarios for consistency with available field observations.
5. To evaluate the effects of repository thermal loading on ambient conditions within the mountain, including in-place fracture and matrix thermodynamic conditions, perched water conditions, gas, moisture and heat flow within and around faults, and hydrological impacts on mineral assemblages.

6. To evaluate the impact and effects of climate change on all ambient and thermally-induced states of the repository region.

During FY1996 much progress was made in the development of the UZ model. Calibrations of the model included matching saturation and water potential data (Chapter 3), gas pressures and flow (Ahlers et al., 1996), ambient temperature and heat flow data (Chapter 9), perched water bodies (Chapter 7) and environmental isotopes (Chapter 11). Work has started on model calibrations with respect to percolation flux rates inferred from fracture coating data (Chapter 14). Coupled calibrations of various state variables have also been started, and these show promising results in terms of better parameter constraints (Chapters 11 and 12). In addition to model calibration, considerable effort was devoted to parameter uncertainties and sensitivity studies for fracture and matrix properties (Chapter 3), infiltration patterns, fault properties and percolation flux (Chapter 8) and fracture and matrix heterogeneities (Chapter 11). Finally, a study of the various numerical approaches (e.g. effective continuum method, dual-porosity, dual-permeability etc.) and their appropriate use for different processes including moisture, gas, heat and chemical flow and transport are presented (Chapter 6), and the development of computer codes (Chapter 4) and the numerical grids (Chapter 5) are described.

In this chapter the conceptual model the unsaturated zone (UZ) is presented, the UZ model is briefly described and the methodology used for its calibration is discussed. Finally, an executive summary of the work performed in FY96 is presented. It should be noted that there is not a total consistency between all of the chapters in terms of some of the parameter values used, because various work components by other participants were not received by LBNL until recently. As this chapter is basically a summary of analyses performed in the other chapters, each of which designates the QA status of data software and conclusions, the QA information will not be repeated here.

1.1 Conceptual Model of the UZ

1.1.1 Conceptual Model Development

In this section we will briefly discuss the conceptual model of the UZ; a detailed conceptual model report is being developed (Kwicklis et al., 1996, in prep.). The conceptual model presented here is a summary of what we believe is the general conceptual model currently used by the Project. Some aspects of the conceptual model are contradicted by the results of the present study; this is further amplified in section 1.5.3.

The current conceptual model is a variation of the basic ideas presented by Montazer and Wilson (1985). Since then the majority of the data collected has been in general agreement with these ideas and concepts. Perhaps the major new data set that causes a significant variation to the conceptual model by Mon-

Figure 1.1.1
A Schematic Cross Section through Yucca Mountain showing Various Conceptual Model Data and Processes.

Subsurface hydrologic processes at Yucca Mountain occur in an arid environment with heterogeneous layers of anisotropic, fractured volcanic rocks (Scott and Bonk, 1984). The volcanic rocks consist of alternating layers of welded and nonwelded ash flow and air fall tuffs. The primary geologic formations found at Yucca Mountain, beginning from the land surface, consist of the Tiva Canyon, Yucca Mountain, Pah Canyon, and the Topopah Spring Tuffs of the Paintbrush Group. Underlying these are the Calico Hills Formation, and the Prow Pass, Bullfrog, and Tram Tuffs of the Crater Flat Group (Buesch et al., 1995). Each of these formations is underlain by an associated nonwelded bed-

ded tuff layer. The geologic formations have been divided into hydrogeologic units (Montazer and Wilson, 1984) based roughly on the degree of welding. These are the Tiva Canyon welded (TCw), the Paintbrush nonwelded (PTn, consisting primarily of the Yucca Mountain and Pah Canyon members and their bedded tuffs), the Topopah Spring welded (TSw), the Calico Hills nonwelded (CHn), and the Crater Flat undifferentiated (CFu) units.

The welded units typically have low matrix porosities and high fracture densities, whereas the nonwelded and bedded tuffs have relatively higher matrix porosities and lower fractures densities (Montazer and Wilson, 1984). At smaller scales, the fracture density is correlated with increases in the degree of welding of the volcanic rocks. Portions of these units can be altered to zeolites or clays depending on their cooling history and the presence of groundwater and heat.

Alteration does not affect porosities greatly but decreases permeabilities of the formations where it occurs (Rousseau et al., 1996). Secondary mineralization of the glassy component of the tuff is characterized by zeolitic alteration (Loeven, 1993). Therefore, altered tuffs are not a significant component in portions of the tuffs where significant welding or vapor-phase alteration during cooling occurred and reduced the glass content of the matrix. Differences in the amount of zeolites in the various pyroclastic and bedded tuff units may be due to variations in their content of primary glass (Bish, 1988; Bish and Chipera, 1989).

The representation of vertical heterogeneities of geology and alteration history at Yucca Mountain in the UZ model is described in Chapter 2 (Bandurraga, 1996).

**1.1.3
Infiltration**

Infiltration at Yucca Mountain is spatially variable due to variations in soil cover and topography. It is also temporally variable due to the nature of the storm events that supply the precipitation (Hevesi et al., 1994). The current conceptual model for infiltration is based on numerous measurements of water content profiles in shallow boreholes at Yucca Mountain. If there is a significant thickness of alluvium overlying the fractured volcanic rock, an infiltration pulse will not penetrate to the volcanics because of attenuation of the pulse by storage in the alluvium. Therefore, infiltration is high on sideslopes and ridgetops where outcrops are exposed and fracture flow into the volcanics can be initiated (Flint and Flint, 1994).

Measurements of water content profiles in the UZ after precipitation events (Hevesi and Flint, 1993) show that infiltration pulses are transient events. However, it is unclear how to represent the temporal variations in precipitation for model input. Also, modeling studies have shown that infiltration pulses are dampened as they proceed through the unsaturated zone, so that close to steady-state conditions in the TSw are found in the matrix (Wang and Narasim-

han, 1985). Therefore, to avoid the uncertainties associated with temporally varying infiltration patterns, the assumption is usually made that infiltration can be characterized with maps that provide steady-state infiltration rates. Several different spatially variable infiltration maps have been developed by project scientists (Hevesi et al., 1996, in prep.; Flint et al., 1996, in prep. Other maps have been developed (A. Flint, USGS, personal communication, January, 1996) which provide long-time scale temporally variable maps showing historic variations in precipitation due to pluvial periods.

1.1.4
Percolation Flux

The percolation flux at the level of the proposed repository in the middle non-lithophysal portion of the TSw is one of the most critical aspects of the site that can be investigated through the use of the UZ model. Data exist to suggest that the flux reaching the repository level through the matrix is relatively small. These data include:

Relatively low matrix saturations measured in the upper portion of the TSw which suggest that much of the moisture which infiltrates into the TCw does not reach the TSw (Flint, 1996, in prep.). Furthermore, the low saturations suggest that fracture flow cannot be maintained through this region.

Data from the ESF show that no weeping fractures were found, even in the region where perched water is found in boreholes (Rousseau et al., 1996). Furthermore, no moisture was observed infiltrating into the radial boreholes of Alcove 1 of the ESF after storm events, even though the boreholes are located close to the land surface in the highly fractured and broken TCw formation (G. LeCain, USGS, personal communication, September 1995).

The relatively high porosities of the units in the PTn attenuate infiltration pulses through storage, possibly allowing vapor transport through the relatively permeable TCw to remove a significant portion of the moisture before it reaches the TSw.

Fracture coating data suggest that if the coatings are continuously deposited the percolation flux is very low (Peterman et al., 1996)

However, other data suggest that the percolation flux may reach the repository level mainly through episodic fracture flow. These data include observation and testing of extensive bodies of perched water located below the repository horizon (Burger and Scofield, 1994). Measurements of bomb-pulse isotope levels in samples from the tuff matrix (Yang, 1996) and the ESF (Fabryka-Martin et al., 1996), show that the water is relatively young. This indicates shorter travel times than would be possible solely through matrix flow. The isotopic data will be discussed in more detail in a later section (see Chapter 10).

Additionally, an analogue site at Rainier Mesa with average annual precipitation approximately double that of Yucca Mountain is reported to have about

23.7 mm/yr infiltrating deep into the subsurface through fault or fracture flow (Wang, 1993). Based on this evidence, a significant portion of the moisture that is estimated to infiltrate into the TCw may reach the repository horizon.

**1.1.5
Lateral Flow**

The infiltration maps predict that significant amounts of infiltration can occur at various locations across Yucca Mountain. There is believed to be a capillary barrier between the welded TCw and underlying PTn which prevents the infiltrated water from penetrating into the PTn (Moyer et al., 1995). Moisture is thought to be diverted laterally through the TCw fractures, following the dip of the geologic formations until it intercepts a fault or a fracture which provides an avenue for downward flow.

This mechanism requires the existence of an abrupt and laterally continuous contact between the TCw and PTn and also that the TCw and PTn have very different hydrologic characteristics. Recent studies in the ESF have shown that the contact can be gradational, and that there are numerous small faults with minor offsets which interrupt the contact's lateral continuity (L. Flint, USGS, personal communication, April 1996). It is difficult to represent this gradational contact which is variably offset in numerical grids. Therefore, it is possible that the significant lateral diversion of flow at the TCw-PTn contact shown in several modeling studies could be an artifact of the numerical grid and the choice of the matrix and fracture properties used in the modeling efforts.

**1.1.6
Effects of Major Faults**

The proposed repository area is surrounded and crossed by numerous strike-slip and normal faults with varying amounts of offset (Scott and Bonk, 1984). The Ghost Dance fault in the repository area has offsets of tens of meters (Spengler et al., 1993), while the Solitario Canyon fault located to the west has offsets of up to hundreds of meters. Modeling studies have been done assuming the faults to be either capillary or permeability barriers (Wittwer et al., 1995), although the evidence for either situation is mixed as illustrated below.

Pneumatic data for NRG-6 (Rousseau et al., 1996) shows that the Drill Hole Wash fault appears to block the effect of the ESF from the sensors deep in the TSw (Ahlers et al., 1996). In this case, gas flow might be blocked by low permeability fault gouge material of the strike-slip fault. Alternatively, the fault may consist of a high porosity zone which attenuates the signal from the ESF in much the same way as the PTn attenuates the atmospheric signal transmitted through the TCw. In contrast, the pneumatic data from UZ-4 and UZ-5 indicate the presence of a fault with a very high lateral permeability connecting these boreholes to the ESF. However, the fault has a relatively low vertical permeability from the TSw to the surface (Ahlers et al., 1996).

Studies in Alcove 2 of the ESF indicate that the permeability of the Bow Ridge fault is about $2\text{E-}11\text{ m}^2$ or about the same as measured with air-k testing

of highly permeable bedded tuff formations or highly fractured welded units (G. LeCain, USGS, personal communication, April, 1996). Also, data from Nye County's borehole ONC#1 (N. Stellavato, Nye County, personal communication, August 1995) shows that the geothermal temperature profile is offset by several degrees as the borehole passes through the Bow Ridge fault zone. This indicates that the fault may be highly permeable to gas or moisture flow which decreases the temperature in that region.

Additional evidence supports the conclusion that the faults may serve as permeability barriers. For instance, the water body observed at borehole SD-7 is thought to be perched over a zeolitic layer and prevented from lateral movement by the presence of the Ghost Dance fault (R. Luckey, USGS, personal communication, September 1995). Rousseau et al. (1996) presented a similar hypothesis that the perched water body intercepted by borehole UZ-14 is caused by a Solitario Canyon fault splay which has offset the zeolitic Calico Hills Formation and blocks lateral movement of the water.

Borehole sensors measuring pneumatic pressures in borehole UZ-7a (preliminary data from J. Rousseau, USGS) appear to show a degree of anisotropy in the fault which is consistent with a permeability barrier, at least in the horizontal direction (Ahlers et al., 1996). Sensors in the fault show little attenuation of the atmospheric signal with depth. The sensors in the TSw adjacent to the fault, however, do show an attenuated signal. Because the TSw has numerous fractures and should be highly permeable to gas, this means that the atmospheric signal in the fault is being blocked in the lateral direction.

Another indication that some faults at the site may act as permeability barriers is obtained from potentiometric surface measurements. Based on these measurements, the potentiometric surface elevation on the western side of the Solitario Canyon fault is approximately 40 m higher than the surface on the eastern side of the fault (Tucci and Burkhardt, 1995). This gradient could only be maintained if the Solitario Canyon fault is somehow a permeability barrier to flow.

**1.1.7
Perched Water**

The presence of perched water has implications for the travel times and flow paths of water through the unsaturated zone, and may affect the construction, operation, and performance of the repository. Perched water may occur where large-permeability differences exist between adjacent geologic formations. Perched-water zones at Yucca Mountain were reported by Burger and Scofield (1994) in the following boreholes: USW UZ-1, USW UZ-14, USW NRG-7/7a, and USW SD-9. Additionally, wet zones were reported to be found in borehole USW SD-12 (C. Rautman, SNL, personal communication, December 1995). Several pumping tests were conducted in borehole UZ-14 and water levels recovered completely after 5.6 days (Burger and Scofield, 1994; and Czarnecki, 1995). This suggested that there is an extensive perched-water body

around this area. In contrast, pressure transient tests of the perched water zone around SD-7 indicate a very limited volume of water.

The perched water bodies or wet layers in these boreholes were detected in zones in or overlying geologic units which are extensively altered to zeolites. This condition is often encountered in the material underlying the densely welded and fractured TSw. Figure 1.1.2 shows the elevations of the perched water reported for all of the boreholes discussed above projected to a north-south cross-section. The figure also shows the top elevation of the nearest underlying zeolitic layer in the borehole. The figure displays the importance of the altered units in creating the perched water zones.

Figure 1.1.2
Perched Water Elevation Data

Qualified zeolitic permeability data from Flint (1995) from boreholes SD-9 and UZ-16 range from about $1\text{E-}18\text{ m}^2$ to the lower limit of the instrument measurement range, $1\text{E-}21\text{ m}^2$. Of the Q zeolitic samples, the lowest log-means (near the instrument lower limit) were obtained with samples from the zeolitized bedded tuff underlying the Calico Hills Formation. Non-Q permeabilities from Loeven (1993) for unaltered samples average about $4\text{E-}16\text{ m}^2$. The low permeability of the altered material is one reason that perched water bodies form above the layers when lateral movement is prevented.

1.1.8 The Effect of Zeolites on Repository to Water Table Flow Paths

A contour map of the distance above the water table for the surface where zeolites are first encountered below the base of the TSw is given in Figure 1.1.3. Assuming that the zeolitic surface serves as a barrier to vertical flow and causes

lateral diversions and perching, the figure shows that perched water north of Drill Hole Wash would be diverted in a southerly direction until it encounters a minimum along the alignment of Drill Hole Wash. Figure 1.1.4 shows a vertical cross-section along UZ-14 and NRG-7 of the hydrogeologic units and altered CHn.

Moisture flow south of Drill Hole Wash would be diverted in an easterly direction unless it is blocked by the Ghost Dance fault. The bottom of the TSw is below the measured potentiometric surface near the western side of the Bow Ridge fault, indicating that fracture flow in the TSw in this region can reach the water table without moving through an extensively altered zeolitic layer.

Figure 1.1.3
Isopach Contour Map of the Thickness of Zeolitic Zone Above Water Table. IN COLOR. Purple contours correspond to top of Calico Hills Formation Zeolites. Green contours correspond to top of Prow Pass zeolites below middle welded devitrified zone (unaltered). Proposed repository blocks shown in yellow. Zones where altered layers intercept water table shown in green.

Figure 1.1.4

Southeast to northwest cross section showing the conceptual idea of perched water on top of the zeolitic Calico Hills unit.

In the southern portion of the proposed repository and southward, parts of the Calico Hills Formation and the Prow Pass Tuff are vitric as shown in the borehole logs of UZ-6 and H-3. The first altered unit which could serve as a barrier to vertical flow is the lower Prow Pass. However, this layer is reported to be subject to less alteration than the Calico Hills Formation and may not impede or laterally divert flow to the same extent as the Calico Hills altered pyroclastic layers. Saturation profiles for the lower Prow Pass in borehole SD-7 (Q data from L. Flint, USGS) show saturations average about 95% while the altered Calico Hills Formation saturations are close to 100% (see saturation profile in Chapter 3, Bandurraga et al., 1996).

Figure 1.1.3 also presents the contours for the distance above the water table for the lower altered Prow Pass surface (Moyer and Geslin, 1995). The gradient of this surface is generally easterly. The devitrified upper Prow Pass intercepts the water table along a west-northwest trending trace passing near UZ#16. If vertical moisture flow is diverted laterally by the lowered altered layer and if the Ghost Dance Fault does not block the flow or provide an alternate pathway to the potentiometric surface, then lateral flow in the devitrified layer will reach the surface in that region without proceeding through a zeolitic layer. No perched water was found overlying the lower altered Prow Pass layer in bore-

hole SD-7 (C Rautman, SNL, personal communication, December 1995). This could be due to several different factors, including: 1) the lower Prow Pass layer in this region is not altered sufficiently to cause perching, 2) the Ghost Dance fault is not creating perched water by blocking laterally diverted flow in this region, or 3) the Ghost Dance fault is serving as an alternate pathway to the potentiometric surface.

1.1.9
Fluid (Water and Gas) Flow
Paths and Ages

A number of isotope measurements are being performed on perched water zones samples, matrix pore water samples, and matrix samples obtained from the unsaturated zone at Yucca Mountain. In addition, fracture coatings and fillings have been tested for isotope concentrations. These isotope measurements can provide an estimate of the age of the samples if the historic atmospheric isotopic concentrations are sufficiently known. Other factors which can affect ages are bomb-pulse concentrations and processes like deposition, sampling effects, dilution, and molecular diffusion.

Recent work on fracture coatings from the ESF have not shown any age estimates younger than about 54 ky, with a majority of the samples falling into the 90-200 ky range (Paces, 1996). However, little is known about the mechanisms of deposition of fracture coatings. There is some evidence to suggest that deposition may occur in tiny 'islands' on the coating surface. Therefore, the sampling procedure may not be able to isolate only the youngest material, and may be biasing the measurements on the side of longer ages.

Some of the recent matrix samples taken from the ESF and in boreholes show the presence of elevated ^{36}Cl in the PTn and upper TSw (Fabryka-Martin and Liu, 1995; Fabryka-Martin et al., 1996). One hypothesis for the elevated ^{36}Cl signals is that they are due to bomb-pulse infiltration, indicating relatively fast transport from the surface compared to matrix flow. One possible mechanism for this phenomenon is that it is associated with transient episodic flow through localized structural features which can penetrate into the TSw and proceed to depth in the fractures (see Chapter 10).

Preliminary data from isotope testing of perched water samples from boreholes UZ-14 and SD-7 indicates that the water had about 28% modern ^{14}C , with an apparent residence time since infiltration of 10,800 years. The corrected age was bounded by a range of 5,000 to 10,800 years, and the samples may be a mixture of different ages (Personal communication, R. Luckey, September 1995).

1.1.10
Geothermal Gradient

The geothermal gradient at Yucca Mountain is relatively well-established and understood through numerous temperature and heat flow measurements. The data include borehole temperature profiles (Sass et al., 1988), surface and water table heat flows, and recent ESF temperature measurements. Deviations from the expected relatively constant slope of the measured temperature gradients from the water table to the land surface are readily explained in terms of

gas and/or moisture flow patterns and thermal conductivity variations. The boundaries of the site-scale model are set based on temperature measurements at the water table and land surface. Past calibration efforts (Ahlers et al., 1995) evaluated the thermal conductivities required to match the measured temperature profiles. However, Rousseau et al. (1996) incorporated an analysis of temperature data in their report which linked variations in the geothermal gradient to infiltration rates. This approach yields some interesting conclusions about percolation fluxes at Yucca Mountain and is discussed in Chapter 9.

1.2 UZ Model and Work Elements in FY96

During FY96 work was performed on most if not all aspects of the UZ model, with the goal that a fully integrated comprehensive model would be completed in June 1997 using all available data for use in Total System Performance Assessment (TSPA) for the Viability Assessment. This report, therefore, only represents a stepping stone in the development of the model, and there are large disparities in the progress made in individual model areas. Some parts of the model are quite mature and will only need updating in FY97, whereas work in other areas has just started. A major effort in FY97 will be to put all of the model pieces and components together in an integrated, comprehensive and defensible UZ model.

1.2.1 Geology and the Numerical Grid

The geological framework underlying the model in terms of stratigraphy, layering and faulting is consistent with the Reference Information Base (RIB) Section 1.2(a), "Stratigraphy: Geologic/Lithologic Stratigraphy" and the Prototype Three-Dimensional Framework model (YW85) of September 1995. Contour maps for many of the sublayers for the extended model boundaries compared to the original Wittwer et al. model were developed; the sublayers were selected based upon moisture tension, saturation, temperature, pneumatic and other data in addition to insights gained from prior modeling and analysis (Wittwer et al., 1995; Ahlers et al., 1995a, 1995b). The numerical grid used in the UZ model utilizes the vertical sublayering from the geological model. Horizontal grid selection is based on many factors, including locations of boreholes, major faults, the Exploratory Studies Facility (ESF), proposed boreholes, infiltration patterns, the potential repository area and locations of proper model boundaries. The main UZ model grid is bounded to the east by Bow Ridge Fault, extends 1 km west of the Solitario Fault and extends approximately from borehole G-2 in the north to borehole G-3 in the south. This grid has about 27,000 grid blocks and about 100,000 connections for Effective Continuum Method (ECM) computations and about 44,000 grid blocks and 165,000 connections for dual-porosity or dual-permeability calculations.

**1.2.2
Initial and Boundary
Conditions; Model
Assumptions**

The 3-D UZ flow model boundaries are provided to simulate the ambient hydrological conditions across the mountain. The top boundary is the top of the Tiva Canyon hydrogeologic unit (TCw), as the alluvium cover is neglected, and the bottom boundary is the water table. Various boundary conditions are prescribed at these boundaries depending on the case considered. In most cases, a constant temperature, air pressure, and infiltration rate is prescribed at the ground surface; these may be spatially variable. In other cases a pulse of water may be imposed at the ground surface. Generally, spatially variable constant temperatures and pressures are prescribed at the water table. In some of the thermal loading studies presented in Chapter 13 the model is extended vertically 500 m into the saturated zone.

The side boundaries of the model are assumed to be no-flow boundaries. Due to the dip of the geological layers, the dominant direction of the lateral flow component is toward the Bow Ridge fault. The breccias and disturbed tuffs in the fault zone are assumed to act as capillary barriers, thus leading to the no-flow boundary assumption.

Specific boundary conditions and modeling assumptions used in the simulations done for these reports are discussed in the individual chapters. For instance, boundary conditions used in 1-D dual permeability model studies are described in Chapter 6 (Doughty et al., 1996). Specific boundary conditions used in perched water evaluations, the 3-D model runs, and the temperature calibration and analysis are provided in Chapters 7 (Wu et al., 1996), 8 (Wu et al., 1996), and 9 (Bodvarsson et al. 1996), respectively. Most of the simulations described in this report are run to steady-state conditions. For transient simulations, the studies are usually started with a model at steady-state conditions and then the transient conditions are imposed as a pulse or step change.

**1.2.3
Rock Properties**

The rock property set used in the UZ flow model described in Wittwer et al. (1995) was a "best-estimate" property set based on limited non-Q data from outcrop studies conducted by Flint and Flint (1992). The matrix van Genuchten parameters were combined with assumed fracture relative permeability curves to be used in the Equivalent Continuum Model (ECM) approach. The property set was not calibrated until the FY95 studies described in Ahlers et al. (1995a).

For FY96, the ECM approach in the UZ flow model was modified to account for flow in fractures and matrix with separate permeability and van Genuchten parameter sets. A set of Q matrix properties (permeabilities and van Genuchten parameters) were developed from data sets generated by L. Flint of the USGS. The latest data from the USGS includes a set of effective geologic layer matrix properties which will be Q in September, 1996 (Flint, 1996, in prep.). These data were concluded to be the best available matrix properties available and were used in the saturation and water potential calibration efforts described in Chapter 3 (Bandurraga et al., 1996). The effect of heterogeneities in the matrix prop-

erty set has been evaluated in modeling studies described in Chapter 11 (Sonnenthal et al., 1996).

**1.2.4
Computer Codes and
Numerical Approaches**

Several new computer codes and modules were developed for the UZ model studies. A generalized Effective Continuum Method (ECM) formulation based on the work of Pruess (1985) was incorporated into the TOUGH2 simulator. This module calculates separate matrix and fracture flow at all saturations. A single-component gas flow module was developed and incorporated into the TOUGH2 code. This module allows the user to solve the flow equation for gas, without the additional water and heat flow equations. The main utility of the "gas flow only" is for the pneumatic pressure simulations reported by Ahlers et al. (1996). Finally, an additional radionuclide transport module was incorporated into TOUGH2 for the analysis of ^{36}Cl . This module rigorously considers radionuclide transport by molecular diffusion, advection and hydrodynamic dispersion. A numerical study was conducted comparing the different numerical approaches (ECM, dual-porosity, dual-permeability, single or multiple matrix blocks etc.) for different processes and problems considered in the UZ model (Chapter 6, Doughty et al., 1996). The results of these studies are intended to guide the development of the UZ model and submodels by ensuring that the most accurate and efficient numerical approach is used for each given problem.

**1.2.5
Model Calibration Activities**

A major effort was devoted to calibration of the UZ model using saturation and moisture tension data, gas flow and pneumatic data (this is discussed in an associated report by Ahlers et al., 1996), temperature data, perched water data and information on environmental isotopes. The saturation and moisture tension data from boreholes were used to calibrate rock matrix and fracture properties using as initial estimates rock property measurements from L. Flint (1996) and the inverse numerical code ITOUGH2 (Finsterle, 1993). The calibration and inverse modeling was performed using various infiltration estimates and fracture and rock matrix parameter values were obtained for each case. The temperature and heat flow data reported by Sass et al. (1988) and Rousseau et al. (1996) were analyzed using two models, the first one a conduction-only model and the second one a coupled conduction/convection model. The UZ model was calibrated against perched water data including locations of perched water, estimated volume and pressure transient test responses and the estimated residence time of the perched water. Preliminary analysis of occurrences and concentrations of environmental isotopes, especially ^{36}Cl , were conducted using two-dimensional models and various conceptualizations. Efforts were concentrated on predicting other occurrences in the remaining parts of the ESF and to evaluate factors affecting the spreading of the ^{36}Cl "bomb-pulse" in the Topopah Springs unit. Finally, initial studies incorporating fracture coating data into the UZ model to help determine or bound the percolation flux were started.

**1.2.6
Coupled Process
Calibrations and Analysis**

Most of the calibrations were conducted using one- or two-dimensional submodels of the UZ-model and usually only considered a single process, for example moisture flow or gas flow. Several studies were performed that considered several processes and compared the simulation results to the observed data. An east-west cross-section through boreholes UZ-6, SD-7 and UZ#16 was developed and the simulation results compared to saturation and moisture tension data from SD-7 and UZ#16, pneumatic data from SD-7, perched water ages in SD-7 and the occurrence of tritium in UZ#16. This model considered a dual-permeability formulation with a pulse of water moving through the system and evaluated the pulse movement through the unsaturated zone. The three-dimensional UZ model is currently calibrated using much of the available data and will hopefully be fully calibrated for several conceptual models in June, 1997.

**1.2.7
Sensitivity Analyses**

Several sensitivity analyses were performed in FY96 using the UZ model and submodels. The numerical errors introduced by the relatively coarse grid used in the UZ model were investigated by grid discretization studies and comparing results in terms of flows and state-variables. A submodel of the UZ model was developed consisting of 10 m grid blocks and the results for percolation flux were compared to that of the UZ model. A brief study including heterogeneities in fracture and matrix permeabilities was then introduced and the percolation flux variability at the repository horizon was evaluated. The UZ model was used for various sensitivity studies involving different infiltration maps and various conceptual models for faults. The UZ model was also used to simulate a climate change scenario using a dual-permeability numerical formulation. Various other sensitivity studies were performed using submodels such as with ^{36}Cl studies, rock and matrix property evaluations, and the evaluation of thermal loading. The thermal loading studies evaluated both the ECM and the dual-permeability formulations using a north-south two-dimensional cross section.

**1.2.8
Model Predictions**

Predictions made with the UZ site-scale model during FY95 were provided in the Ahlers et al. report (1995b). The predictions were made for the portions of boreholes SD-12 and SD-7 which had not been evaluated for core sample saturations and water potentials by the time the report was published. The predictions were also done for borehole ONC#1 and UZ-7a. Temperature predictions were also done for these boreholes. At this time, no new boreholes have been drilled at Yucca Mountain during FY96 and therefore no new blind predictions are provided in this report. However, many of the chapters provide comparisons between model predictions of state variables and observed borehole data.

Predictions of the pneumatic pressure response in boreholes due to the construction of the ESF have been performed at regular intervals and provided to USGS researchers during FY95 and FY96. Comparisons of the predictions and subsequently measured data have developed confidence in the ability of the UZ

model to characterize gas flow patterns and pressures at Yucca Mountain. The prediction process and comparison is provided in the pneumatic data analysis milestone which accompanies this report (Ahlers et al., 1996). Predictions of various state variables throughout the three-dimensional model domain is given in various chapters, especially Chapters 7 (Wu et al.) and 8 (Wu et al.). For example, these predictions can be used to predict the saturations, temperature and moisture conditions in the rocks that will be encountered in the south ramp of the ESF. Another example is a prediction of the expected locations of "bomb-pulse" ^{36}Cl , given in Chapter 10 (Fairley et al.).

1.2.9**Model Uses and Limitations**

As discussed in the introduction to this section, this report represents a stepping stone in the development of the model. Some parts of the model will only need updating in FY97, whereas work in other areas has just started. A major effort in FY97 will be to integrate all of the model components. The model, as it is presently formulated, is intended to be used to simulate ambient conditions in the unsaturated zone at Yucca Mountain as they are represented by borehole data and site study results. It can also be useful in sensitivity analyses and predictive work studying variations in boundary conditions and thermal loading scenarios; however, no data are presently available to calibrate the model for these purposes. The model is limited in general by the uncertainties associated with the parameter sets used in the analyses, and the quantity of data available for model calibration. Modeling results and conclusions are also limited based on the boundary conditions and assumptions used in the simulations. Before an integrated model is developed for FY97, the analyses presented in this report include the following specific limitations:

- The geologic model developed in Chapter 2 is not well-constrained in the extended model areas away from the vicinity of the proposed repository due to the limited borehole log data. This is especially true for the model area to the north of Yucca Wash. Additionally, the transition zone between the altered and unaltered zones in the Calico Hills Formation is not well-defined. Study results dependent on the altered layer to provide perched water conditions in this transition area have associated uncertainties due to this.
- The rock property calibration presented in Chapter 3 has associated uncertainties due to the limited data available for calibration as discussed in the chapter. Therefore, the results of modeling studies and conclusions based on the use of the property sets developed in that chapters are subject to uncertainties. The calibration assumed that infiltration rates were temporally constant during the steady-state runs, and the effects of using the parameter sets with infiltration pulses have not been evaluated. The calibration using coupled data sets is in progress, but the results are not reported in these chapters.
- The modeling codes presented in Chapter 4 are subject to the same general limitations typical for numeric methods representing complex unsaturated zone processes. The conceptual models with which the methods are used must be evaluated carefully for their applicability. The numeric grids developed in Chapter 6 are subject to grid dispersion and diffusion errors associated with numerical models of heterogeneous geologic systems. The aspect ratio in some of the grid blocks can be quite large, and

the number of layers in the UZ model can characterize only broad variations in hydrological properties. It is not intended to be used to represent very small-scale subsurface variations.

- The perched water studies of Chapter 7 assumed that steady-state conditions existed. The travel time estimates provided are based on particle tracking calculations and do not take into account temporal variations in infiltration rates or complex mixing or diffusion phenomena. The results of the analyses of Chapters 7 through 14 are dependent parameters sets used in the analyses for the matrix, fractures, and faults. They are also dependent on the limitations and uncertainties associated with the data sets used in the analyses.
- The temperature analysis results presented in Chapter 13 provided temperature predictions for close to the top of the model near the ground surface. The model top is not coincident with the land surface due to gridblock size and presence of alluvial layers. Therefore, the temperatures predicted for the model top should not be construed to represent actual land surface temperatures.

1.3 Summary and Conclusion of FY96 Work

A new version of the UZ model was developed in Fiscal Year 1996 which built on previous UZ models (Wittwer et al., 1995; Ahlers et al., 1995a, 1995b). This new version of the model contains more geologic realism and accuracy in representation, using almost 30 computational layers as the basis for the numerical grid. The grid is refined in the repository area to allow for more accurate determination of flow patterns and directions. The model contains most, if not all, important processes and components of the mountain, including faults and fault offsets, perched water in appropriate locations, rock matrix and fracture properties that correspond to saturation and moisture tension data and various infiltration maps, observed temperature profiles from boreholes and fast flow paths as observed through environmental isotopes. The calibration of the model proceeded using various one- and two-dimensional submodels for individual processes and the resulting parameter values were incorporated into the three-dimensional model. A study of various numerical approaches (e.g. Effective Continuum Model (ECM), dual-porosity, dual-permeability, and single-versus multiple-matrix block representation etc.) and their accuracy and efficiency in modeling different processes guided the choice of numerical method for the UZ model and submodels. The results of the study show that the ECM method is preferred for steady-state moisture flow and transient gas flow, whereas dual-continua methods are more appropriate for the modeling of transient pulses, transport and thermal loading. This report presents dual-permeability calculations for coupled-process submodel, a climate change scenario using the 3-D UZ model and for thermal loading studies.

The following sections discuss how the important conceptual model elements are affected by the conclusions of the UZ modeling and analysis in FY96.

**1.3.1
Percolation Flux**

One of the main objectives of the UZ model is to determine the spatial and temporal distribution of percolation flux at the repository horizon. This parameter is the most important one for Performance Assessment (PA) and Total System Performance Analysis (TSPA). The percolation flux is a difficult parameter to determine for low flux regions such as Yucca Mountain, and unfortunately there are no reliable direct measurements that can be made to determine this important parameter. Thus, one must rely on a mixture of other indirect methods involving field testing and modeling of various processes at different scales. Our analysis of the available temperature and heat flow data suggest that these data may be helpful in bracketing current values of percolation flux across the repository area (see Chapter 9). The results of the analysis indicate that the average percolation flux in the repository area is on the order of 5 mm/yr. Comparison of this analysis with three-dimensional modeling results of percolation flux at the repository horizon using the latest infiltration map by Flint et al. (1996) indicate very similar results on the order of 5 to 10 mm/yr. This somewhat simple analysis suggests that this range of percolation flux is prevalent over most of the potential repository area between Solitario Canyon fault and the Ghost Dance fault. It is acknowledged that the available data are limited and that the method of analysis has not been proven for this type of analysis. The analysis of the moisture tension and saturation data from the boreholes are not in direct conflict of these average percolation flux values, but they do somewhat favor lower values (see Chapter 3). However, a pulse type infiltration process with high infiltration occurring over short time frames and then low steady infiltration rates over relatively long time periods is consistent with the measured saturation and moisture tension data.

The partitioning of the percolation flux at the repository horizon into fracture and matrix components is of great importance as it will affect the water flow into the drifts. Our simulations using the UZ model indicate that this partitioning depends strongly on the matrix permeability of the middle non-lithophysal unit of the TSw, which is the repository rock. Measurements by L. Flint (1996) yield an average value for this unit of a few micro-darcies, but with a range of six orders of magnitude for one standard deviation. If the effective matrix permeability (parallel conductance average) of the middle non-lithophysal unit is an order of magnitude higher than the current average value (based on only 11 samples), one would expect a predominantly matrix flow in the repository host rock unit. We will investigate this with the 3-D submodel discussed in Chapter 11 using heterogeneities at different scales. Also of interest is the recent fracture coating information. We are in the process of evaluating various options of how to use these data will help us constrain the percolation flux (see Chapter 14, Simmons).

**1.3.2
Lateral Flow in the
Unsaturated Zone**

Three-dimensional analysis of lateral flow using the UZ model suggests that lateral flow within or around the Paintbrush non-welded unit (PTn) is most prevalent at relatively low infiltration/percolation flux rates. The results of the

modeling show lateral flow within the PTn for several kilometers when an average low infiltration rate of about 0.1 mm/yr is applied at the ground surface (see Chapter 8). However, as we currently believe that the average percolation flux over the repository horizon is about 5 mm/yr, the model results predict little lateral flow. The PTn unit is predicted to somewhat average spatial and temporal variability in the infiltration rate, but the previous conceptual model theories of large scale lateral flow within or around the PTn towards major faults is not supported by our modeling results (see Chapter 8). Lateral flow above the low permeability zeolitic rocks within the Calico Hills and the Prow Pass units is seen in most of our two-dimensional and three-dimensional simulations. In addition, the temperature gradient analysis performed in Chapter 9 suggests less vertical percolation flux within the Calico Hills and the Prow Pass layers than the Topopah Springs unit, thereby indicating lateral flow must occur above these layers. Lateral flow above the zeolitic units is a critical issue as the Project determines how much dependence should be placed on retardation and sorption due to flow through the zeolitic rocks.

**1.3.3
Effects of Major Faults**

Currently very limited data are available regarding the flow characteristics of major faults for gas and moisture flow. Temperature data for UZ-7a which penetrates the Ghost Dance fault suggest that the percolation flux within the fault is less, if anything, compared to that of the surrounding fractured porous rock (see Chapter 9). Pneumatic data indicate that most faults are permeable to gas, thereby suggesting that they are not fully saturated with water. The permeability to gas varies widely from high horizontal permeabilities within the TSw unit to relatively poor gas connectivity from the TSw to the ground surface (Ahlers et al., 1996). ^{36}Cl "bomb-pulse" data show fast flow to the repository horizon, mostly associated with major faults. The 3-D model results show relatively higher percolation rates down major faults than through the adjacent fractured rocks, especially for cases with high infiltration rates. In addition, for simulations using the latest infiltration map with an average rate of 4.4 mm/yr in the repository area, lateral flow within and around the PTn is small. Lateral flow beneath the repository may be large above the zeolitic units. Thus, for this case one may expect that faults do not greatly affect moisture flow within and above the TSw, but may have much more of a role within the underlying Calico Hills and Prow Pass layers.

**1.3.4
Fast Flow Paths**

"Bomb-pulse" ^{36}Cl data and tritium data show that fast flow paths exist at Yucca Mountain as these isotopes are found in localized areas in the ESF, mostly near major structures. Our analysis of these data suggest that in most cases major structures are needed to transport fluids and chemicals rapidly through the PTn unit, and that this is most efficiently done by intermittent water pulses. Our favored conceptual model relies on areas within washes with little alluvium cover that are intersected by faults and are prone to flooding. On the basis of this conceptual model and analysis of current occurrences ^{36}Cl in the ESF, we think that there is good chance that "bomb-pulse" ^{36}Cl can be found in the ESF

near stations 50+00, 57+00 to 61+00 and 68+00. It should be noted that "bomb-pulse" ^{36}Cl occurrences at the ESF will not help determine the global percolation flux. Analysis of the ^{36}Cl data in terms of occurrence and spreading can, at best, constrain the pulse strength required to get the isotope to the repository level on a localized scale. Our conceptual model relies on focusing of infiltrated water during storms into structural features. These pulses may be few and far between (every 10 years or so), so that they do not affect the average behavior of the mountain or its "quasi-steady state" flow patterns.

**1.3.5
Perched Water**

The conceptual model discussion involving perched water bodies in section 1.1.7 stressed the importance of zeolitic rocks and the basal vitrophyre of TSW as the perching geological units. The numerical simulations of the perched water zones discussed in Chapter 7 (Wu et al) found that vertically these units had to be of very low matrix permeability (less than a micro-darcy) with little or no fracture permeability in order to produce perched water. In addition, there had to be lateral constraints on water flow by permeability barriers, at least down dip of the expected perched water location. Rousseau et al. (1996) in the North Ramp report use a "hypothetical fault" down dip to provide the perching. We do not constrain our model with such a closed boundary for moisture flow, but rather investigate how low the laterally confining permeability must be to generate perched water under various infiltration scenarios. This permeability turns out to be several hundreds of milli-darcies for the relatively low infiltration scenarios tested in our simulations. This permeability is about an order of magnitude lower than the global large scale horizontal permeabilities inferred from pneumatic testing, and somewhat lower than those inferred from the gas permeability packer tests (LeCain, 1996). Current work suggests that using the latest infiltration map (Flint et al., 1996) will result in horizontal permeabilities necessary for perching that are consistent with the results of the air-permeability testing as well as with the results of the pneumatic testing program. This evidence again supports the hypothesis of 5 to 10 mm/yr percolation flux through the repository horizon.

The simulations using the UZ model resulting in the perched water conditions are consistent with a water residence time of 5000 to 10,000 years. Most of the water flow is through the fractures resulting in relatively short water flow travel times.

**1.3.6
Evaluation of Calibration
Quality of the UZ Model**

A detailed east-west cross-sectional model through boreholes UZ-6, SD-7 and UZ#16 was developed in order to evaluate the quality of the calibration process (see Chapter 12). The cross-section was simulated using a dual-permeability formulation with the latest infiltration map (Flint et al., 1996). The results showed excellent agreement with various data sets including saturation and moisture tension data from SD-7 and UZ#16, pneumatic data from SD-7 and temperature data from UZ-7a and H-3, without any additional calibrations. This submodel also verified to some degree the methodology of determining

the percolation flux from temperature gradient data discussed in Chapter 9. Finally, the submodel investigated the presence of fast flow paths using a pulse at the ground surface.

**1.3.7
Thermal Loading Studies**

Thermal loading studies were conducted using a north-south cross section through the repository region, using both ECM and dual-permeability numerical formulations. A 500 m portion of the saturated zone was included in the model. The results obtained showed that including the saturated zone in the model does not make a major difference, although more realistic estimates for temperature increases in the basal vitrophyre of TSw and within the Calico Hills unit are obtained. Temperature increases of some 5-10°C are expected near the ground surface and about 30°C at the water table, with the maximum temperature increase occurring about 1000 years after emplacement. Heat pipe conditions prevail in the repository horizon, and complete dryout occurs when low infiltration rates (e.g. 0.1 mm/yr) are used. In the case of high-infiltration rates (e.g. 4.4 mm/yr) no dryout occurs. This is very important because this implies 100% humidity which greatly enhances corrosion rates. The ECM and dual-permeability formulations showed similar results for many aspects of thermal loading, but differed mainly in the extent of the boiling zone and the transient water flow through the repository.

**1.3.8
Climate Change Scenario**

A dual-permeability simulation using the 3-D UZ model with a climate change was conducted. It was assumed that the current spatially variable infiltration rates all increased by a factor of three, and the impact on moisture flow within the mountain was evaluated. The results showed that the pulse moves rapidly through the system and reaches the water table in less than 1000 years in many locations. Localized fast paths allow movement through the UZ in tens of years down to the water table. The major barriers to the vertical flow are the zeolitic units in the Calico Hills and Prow Pass and these enhance recharge to the perched water bodies. Rapid fracture flow occurs through the repository horizon. The system reaches steady state after about 30,000 years.

1.4 Acknowledgments

This acknowledgment applies to all chapters of this report. Technical review of this work was conducted by the following technical staff of E.O. Lawrence Berkeley National Laboratory: Chapter 1, C. Doughty and C. Oldenburg; Chapter 2, N. Goldstein and A. Simmons; Chapter 3, T. Tokunaga, and J. Najita; Chapter 4, G. Moridis and E. Schlueter; Chapter 5, A. James and J. Peterson; Chapter 6, A. Cohen and J. Birkholzer; Chapter 7, M. Lippmann and K. Karasaki; Chapter 8, Y. Tsang and M. Lippmann; Chapter 9, C. Doughty and B. Freifeld; Chapter 10, Y. Tsang and K. Karasaki; Chapter 11, Y. Tsang and A. Cohen; Chapter 12, A. James and J. Wan; Chapter 13, Y. Tsang and C. Doughty;

Chapter 14, J. Apps and L. Cox. The careful review and responsiveness of the reviewers is most appreciated. QA reviews of all chapters was conducted by D. Mangold, and his work and responsiveness is most appreciated. The authors acknowledge fruitful collaborations with the following USGS colleagues for their sharing of data and technical expertise: E. Kwicklis, A. Flint, L. Flint, J. Rousseau, G. Patterson, G. LeCain, J. Sass, L. Anna and others. Suggestions by R. Linden as a Technical Reviewer of a QA audit is appreciated. Technical and managerial assistance and collaboration with R. Patterson, D. Hoxie and D. Gillies is acknowledged. Finally, the authors thank M. Fink, J. Gamble, P. Lau, V. Fissekidou, and A. Sweet for producing the document.

This work was supported by the Director, Office of Civilian Radioactive Waste Management, U.S. Department of Energy, through a Memorandum Purchase Order EA9013MC5X between TRW Environmental Safety Systems, Inc. and Ernest Orlando Lawrence Berkeley National Laboratory, under Contract No. DE-AC03-76SF00098.

1.5 References

Ahlers C.F., T.M. Bandurraga, G.S. Bodvarsson, G. Chen, S. Finsterle, and Y.S. Wu, Summary of model calibration and sensitivity studies using the LBNL/USGS Three-Dimensional Unsaturated Zone Site-Scale Model, September, 1995.

ACCN: MOL.19960208.0091-0097

DTN: LB092995312293.001 (Non-Q)

Arnold B.W., S.J. Altman, T.H. Robey, R.W. Barnard, T.J. Brown, Unsaturated-zone fast-path flow calculations for Yucca Mountain groundwater travel time analyses (GWTT-94), Yucca Mountain Site Characterization Project Report, SAND95-0857, UC-814, September, 1995.

Bish D.L., and S.J. Chipera, Revised mineralogic summary of Yucca Mountain, Nevada, Los Alamos National Laboratory Report LA-11497-MS, UC-721, issued March, 1989.

ACCN: NNA.19890126.0207

DTN: LA000000000018.001 (Non-Q)

Bish D.L., Evaluation of past and future alterations in tuff at Yucca Mountain, Nevada, based on the clay mineralogy of drill cores USW G-1, G-2, and G-3., LA-10667-MS, 1988.

ACCN: NNA.19890126.0207

DTN: LA000000000040.001 (Non-Q)

- Buesch, D.C., R.W. Spengler, T. C. Moyer, and J.K. Geslin, Nomenclature and Macroscopic Identification of Lithostratigraphic Units of the Paintbrush Group Exposed at Yucca Mountain, Nevada, Report USGS OFR 94-469, U.S. Geological Survey, 1995.
DTN: GS9312083124211.049 Q
- Burger, P.A., and Scofield, K.M., Perched water at Yucca Mountain - implications on the exploratory studies facility, Nye County, Nevada, Water-Resources Investigations Report 94-xxx, U.S. Geological Survey, 1994.
- Czarnecki, J., Personal communication, 1995.
- Fabryka-Martin J.T., and B. Liu, Distribution of chlorine-36 in UZ-14, UZ-16, perched water, and the ESF North Ramp, Yucca Mountain, Nevada, LANL Milestone Report 3431, 1995.
- Fabryka-Martin J.T., P.R. Dixon, S. Levy, B. Liu, H.J. Turin, and A.V. Wolfsberg, Summary report of chlorine-36 studies: systematic sampling for chlorine-36 in the Exploratory Studies Facility, LANL Level 4 Milestone Report 3783AD, March 29, 1996.
- Finsterle, S., ITOUGH2 User's Guide Version 2.2, Report LBNL-34581, Lawrence Berkeley National Laboratory, Berkeley, CA, 1993.
ACCN: MOL.19941026.0075
- Flint L., Project Data Tracking Number GS950608312231.006. UZ-16 and SD-9 Permeability Data. 1995.
- Flint L., Matrix properties of hydrogeologic units at Yucca Mountain, Nevada, USGS OFR96-xxx, 1996.
DTN: GS950308312231.002 (Q)
- Flint AL, H.A. Hevesi, and L.E. Flint, Conceptual and numerical model of infiltration for the Yucca Mountain Area, Nevada, USGS WRI 96-xxxx, 1996. In prep.
- Flint A.L., L.E. Flint, and J.A. Hevesi, The influence of long term climate change on net infiltration at Yucca Mountain, Nevada, In Proceedings of the Fourth Annual International Conference on High Level Radioactive Waste Management, Las Vegas, Nevada, V. 1, pp. 152-159, 1993.
ACCN: NNA.19930615.0054
- Flint, A.L. and L.E. Flint, A water potential approach to standardize oven dryness, Abstract, U.S. Geological Survey, 1992.
ACCN: NNA.19930128.0010

Flint, L.E. and A.L. Flint, Preliminary permeability and water-retention data for nonwelded and bedded tuff samples, Yucca Mountain Area, Nye County, Nevada, Open-File Report 90-569, U.S. Geological Survey, 1990.

ACCN: NNA.19901015.0200

DTN: GS920108312231.006

Flint, L.E. and A.L. Flint, The influence of long term climate change on net infiltration at Yucca Mountain, Nevada, Proceedings of the Fourth International Conference on High Level Radioactive Waste Management, Las Vegas, NV, April 26-30, pp.152-159, American Nuclear Society, La Grange Park, IL, 1993.

ACCN: NNA.19930615.0054

Flint, L.E., A.L. Flint, and J.A. Hevesi, Shallow infiltration processes in arid watersheds at Yucca Mountain, Nevada, in Proceedings of the Fifth International High Level Radioactive Waste Management Conference, (American Nuclear Society, La Grange Park, IL), Las Vegas, NV, May 22-26, 1994, pp. 2315-2322, 1994.

ACCN: MOL.19950419.0114

Fridrich C.J.; W.W. Dudley Jr., and J.S. Stuckless, (GS920708318325.001) Hydrogeologic analysis of the saturated-zone ground water system, under Yucca Mountain, Nevada, Journal of Hydrology, 154, (1994) 133-168

Hevesi J.A., and A.L. Flint, Geostatistical model for estimating precipitation and recharge in the Yucca Mountain region, Nevada-California, USGS Report WRI96-xxxx, 1996.

DTN: GS960108312111.001 (Non-Q)

Hevesi J.A., and A.L. Flint, The influence of seasonal climatic variability on shallow infiltration at Yucca Mountain, Nevada, Proceedings of the Fourth Annual International Conference High Level Radioactive Waste Management, Sponsored by the American Nuclear Society and American Society of Civil Engineers, Las Vegas, Nevada, 1993.

Hevesi JA, and A.L. Flint, Geostatistical model for estimating precipitation and recharge in the Yucca Mountain region, Nevada-California, USGS Report WRI96-xxxx, 1996. In prep.

Hevesi, J.A., A.L. Flint, L.E. Flint, Verification of a one-dimensional model for predicting shallow infiltration at Yucca Mountain, Proceedings of the Fifth International high-Level Radioactive Waste Management Conference, pp.2323-2332, May 1-4, 1994.

ACCN: MOL.19950419.0112

DTN: GS940200012544.004 (Non-Q)

Ho C.K., Modeling infiltration into a tuff matrix from a saturated vertical fracture proceedings of the Fifth Annual International Conference High Level Radioactive Waste Management, Sponsored by the American Nuclear Society and American Society of Civil Engineers, Las Vegas, Nevada, pp.1897-1904, May 22-26, 1994.
ACCN: NNA.19940629.0073

Kwicklis, E.M., A.L. Flint, and G.S. Bodvarsson, Updated conceptual model of the unsaturated zone of Yucca Mountain, Nevada, 1996. In prep.

Kwicklis, E.M.; A.L. Flint, and R.W. Healy, Simulation of flow in the unsaturated zone beneath Pagany Wash, Yucca Mountain Proceedings, Fifth Annual International Conference High Level Radioactive Waste Management, Las Vegas, Nevada, May 22-26, 1994.
DTN: GS940208312291.001 (Non-Q)

Lecain G.D., and J.N. Walker, Results of air-permeability testing in a vertical borehole at Yucca Mountain, Nevada, Proceedings of the Fifth Annual International Conference High Level Radioactive Waste Management, Las Vegas, Nevada, May 22-26, 1994.
ACCN: NNA.19940829.0015

Liu B, J. Fabryka-Martin, A. Wolfsberg, B. Robinson, and P. Sharma, Significance of apparent discrepancies in water ages derived from atmospheric radionuclides at Yucca Mountain, Nevada, Water Resources at Risk, Denver, CO, American Institute of Hydrology, May 14-18, 1995.

Loeven C, A summary and discussion of hydrologic data from the Calico Hills nonwelded hydrogeologic unit at Yucca Mountain, Nevada, Los Alamos National Laboratory Report LA-12376-MS, UC-814, January, 1993.
ACCN: NNA.19921116.001

Montazer, P. and W.E. Wilson, Conceptual hydrologic model of flow in the unsaturated zone, Yucca Mountain, Nevada, Water Resources Investigations Report 84-4345, U.S. Geological Survey, 1984.
ACCN: NNA.19870519.0109

Moyer T.C., and J.K. Geslin, Lithostratigraphy of the Calico Hills formation and the Prow Pass tuff (Crater Flat Group) at Yucca Mountain, USGS OFR 94-460, 1995.
DTN: GS940608314211.028 (Non-Q)

Nelson PH., Computation of porosity and water content from geophysical logs, Yucca Mountain, Nevada. USGS OFR96-078, 1996.

Paces J., Dating of fracture coatings in ESF, USGS Milestone 3GQH455, February 23, 1996.

- Peterman, Z.E. and J.B. Paces, Paleohydrology - age control from U-series and ^{14}C dating of calcite and opal in the ESF, presentation given to U.S. Nuclear Waste Technical Review Board, Denver, CO, July 9-10, 1996.
- Peterman Z.E., J.S. Stuckless, B.D. Marshall, S.A. Mahan, and K. Futa, Strontium isotope geochemistry of calcite fracture fillings in deep core, Yucca Mountain, Nevada--a Progress Report, Proceedings of the Third Annual International Conference on High Level Radioactive Waste Management, (American Nuclear Society and American Society of Civil Engineers, Eds.), Las Vegas, Nevada, V. 2, pp. 1582-1586, 1992.
ACCN: NNA.19921116.0073
DTN: GS920208315215.009 (Q)
- Rautman, C.A., Modeling spatial heterogeneity of thermal conductivity using a surrogate property, Proceedings of the Sixth Annual International Conference on High-Level Radioactive Waste Management, Las Vegas, NV, pp.83-84, 1995a.
ACCN: MOL.19950321.0080
- Rautman, C.A., Preliminary geostatistical modeling of thermal conductivity for a cross section of Yucca Mountain, Nevada, Report, SAND 94-2283, WC-814, Sandia National Laboratory, Albuquerque, NM, 1995b.
DTN: SNSAND94228300.000 (Non-Q)(Non-Q)
- Robinson B.A., A.V. Wolfsberg, G.A. Zyvoloski, and C.W. Gable, An unsaturated zone flow and transport model of Yucca Mountain, LA-Milestone 3468 (Draft), October, 1995.
- Robison, J.H., Ground-water level data and preliminary potentiometric surface map of Yucca Mountain and vicinity, Nye County Nevada, Water Resources Investigations Report 84-4197, U.S. Geological Survey, 1984.
ACCN: NNA.19920131.0342
- Rockhold, M.L., B. Sagar, and M.P. Connelly, Multi-dimensional modeling of unsaturated flow in the vicinity of exploratory shafts and fault zones at Yucca Mountain, Nevada, Proceedings of the First International Conference on High Level Radioactive Waste Management, Las Vegas, NV, pp.1192-1199, 1990.
ACCN: NNA.19920131.0342
- Rousseau J.P., E.M. Kwicklis, and C. Gillies, ed.s, Hydrogeology of the unsaturated zone, North Ramp area of the Exploratory Studies Facility, Yucca Mountain, Nevada, USGS WRI-96xxxx, 1996. (in print)
- Sass J.H., A.H. Lachenbruch, W.W. Dudley Jr., S.S. Priest, and R.J. Munroe, Temperature, thermal conductivity, and heat flow near Yucca Mountain, Nevada: some tectonic and hydrologic implications, USGS OFR-87-649, 1988.
ACCN: MMA/19890123.001
DTN: GS950408318523.001 (Non-Q)

Scott, R. B., and J. Bonk, Preliminary geologic map of Yucca Mountain, Nye County, Nevada, with geologic sections. Report USGS OFR-84-494, US Geological Survey, 1984.

ACCN: NNA.19890511.0105

DTN: GS930283117461.001 (Non-Q)

Spengler R.W., C.A. Braun, R.M. Linden, L.G. Martin, D.M. Ross-Brown, and R.L. Blackburn, Structural character of the Ghost Dance Fault, Yucca Mountain, Nevada, Proceedings of the Fourth Annual International Conference on High Level Radioactive Waste Management, Sponsored by the American Nuclear Society and American Society of Civil Engineers, Las Vegas, Nevada, pp. 653-659, April 26-30, 1993.

ACCN: NNA.19931025.0021

DTN: GS930108314221.001 (Q)

Sweetkind D.S., E.R. Verbeek, J.K. Geslin, and T.C. Moyer, Fracture character of the paintbrush tuff nonwelded hydrologic unit, Yucca Mountain, Nevada, Draft USGS OFR, 1995.

DTN: GS950808314222.006

Tucci P, and D.J. Burkhardt, Potentiometric-surface map, 1993, Yucca Mountain and Vicinity, Nevada, USGS WRI95-4149, 1995.

DTN: GS950508312312.005 (Non-Q)

Vaniman D.T., Calcite deposits in fractures at Yucca Mountain, Nevada, Proceedings of the Fourth Annual International Conference on High Level Radioactive Waste Management, American Nuclear Society and American Society of Civil Engineers, Eds., Las Vegas, Nevada, V. 2, pp. 1935-1939, 1993.

ACCN: NNA.19931028.0001

Vaniman D., D. Bish, D. Broxton, F. Byers, G. Heiken, B. Carlos, E. Semarge, F. Caporuscio, and R. Gooley, Variations in authigenic mineralogy and sorptive zeolite abundance at Yucca Mountain, Nevada, based on studies of drill cores USW GU-3 and G-3. LA-9707-MS.

ACCN: NNA.19921124.0020

DTN: LA000000000025.001 (Non-Q)

Wang J.S.Y., N.G.W. Cook, H.A. Wollenberg, C.L. Carnahan, I. Javandel, and C.F. Tsang, Geohydrologic data and models of Rainier Mesa and their implications to Yucca Mountain, Proceedings of the Fourth Annual International Conference on High Level Radioactive Waste Management, American Nuclear Society and American Society of Civil Engineers, Eds., Las Vegas, Nevada, V. 1, pp. 675-681, 1993.

ACCN: NNA.19940203.0038

Wang, J.S.Y., Variations of hydrological parameters of tuff and soil, Proceedings of the Third International Conference on High-Level Radioactive Waste Management, Las Vegas, NV, pp.77-731, 1992.

ACCN: MOL.19950223.0067

- Wang, J.S.Y. and T.N. Narasimhan, Hydrologic mechanisms governing fluid flow in partially saturated, fractured, porous tuff at Yucca Mountain, Water Resources. Research, 21, pp.1861-1874, 1985.
ACCN: HQS.19880517.2566
- Wittwer C., G.S. Bodvarsson, M.P. Chornack A.L. Flint, L.E. Flint, B.D. Lewis, R.W. Spengler, and C.A. Rautman, Design of a 3D site-scale model for the unsaturated zone at Yucca Mountain, Nevada, Proceedings of the Third International High-Level Radioactive Waste management Conference, American Nuclear Society, pp.263-71, 1992.
ACCN: NNA.19930119.0139
DTN: GS911208312293.001 (Non-Q)
- Wittwer, C. S., G. Chen and G. S. Bodvarsson, Studies of the role of fault zones of fluid flow using the site-scale numerical model of Yucca Mountain, Proceedings of the Fourth International Conference on High Level Radioactive Waste Management, Las Vegas, NV, pp.667-674, April 26-30, 1993.
ACCN: NNA.19931129.0085
DTN: GS930308312293.002 (Non-Q)
- Wittwer, C., G. Chen, G.S. Bodvarsson, M.P. Chornack, A.L. Flint, L.E. Flint, E. Kwicklis, and R.W. Spengler, Preliminary development of the LBL/USGS three-dimensional site-scale model of Yucca Mountain, Nevada, Report LBL-37356, UC-814, Lawrence Berkeley National Laboratory, Berkeley, CA, 1995.
DTN: GS940908312293.002 (Non-Q)
- Yang I.C., Flow and transport through unsaturated rock -- data from two test holes, Yucca Mountain, Nevada, Proceedings of the Third Annual International Conference on High Level Radioactive Waste Management, American Nuclear Society and American Society of Civil Engineers, Eds., Las Vegas, Nevada, V. 1, pp. 732-737, 1992.
ACCN: NNA.19930112.0137
DTN: GS920908312272.001 (Non-Q)
- Yang I.C., C.A. Peters, and D.C. Thorstenson, Carbon isotopic data from test hole USW UZ-1, Yucca Mountain, Nevada, Proceedings of the Fourth Annual International Conference on High Level Radioactive Waste Management, American Nuclear Society and American Society of Civil Engineers, Eds., Las Vegas, Nevada, V. 1, pp. 401-406, 1993.
- Yang, I.C., G.W., Rattray, and P. Yu, Interpretations of chemical and isotopic data from boreholes in the unsaturated zone at Yucca Mountain, Nevada, U.S. Geological Survey Water Resources Investigations Report 96-4058, 58+ pp., 1996.

GEOLOGICAL MODEL DEVELOPMENT AND VERTICAL LAYERING SCHEME FOR THE NUMERICAL GRID

T.M. Bandurraga

August 1996

2.1 Introduction

The complexities in geological layering, extensive faulting, highly variable offsets along faults, and hydrogeologic interaction between layers and with the ground surface and the water table make the geological grid development a formidable task. All of the above factors can have large effects on flow patterns of moisture, gas, and heat as represented in a numerical grid of a site-scale unsaturated zone model (UZ model). On the other hand, including all heterogeneities at different scales is not feasible, so careful decisions must be made as to what features to include in the model.

In the vertical direction, heterogeneities are largely due to the depositional environment of the ash flow and air fall tuffs found at Yucca Mountain. Flow cooling led to fracturing, welding, secondary mineral alteration and formation of lithophysal cavities which affect subsurface flow. The hydrothermal and tectonic environment after deposition led to additional fracturing, alteration, and faulting which further affects flow processes in the UZ. The geological studies and borehole drilling efforts have provided numerous data on the extent and intensity of these variations in the subsurface.

Geological models of Yucca Mountain have been developed previously. Some of the first models were presented by the staff of Sandia National Laboratories (Nimick and Williams, 1984; Ortiz et al. 1985). These models presented cross-sections and a limited number of isopach maps of important geological formations. Ortiz et al. included a map which defined the distance to the zone of prevalent alteration below the basal vitrophyre of the Topopah Spring Tuff.

Wittwer et al. (1992) then used additional borehole information and geological studies to develop a geological model which could be used to generate numerical grids for the first site-scale UZ model. The model consisted of structure contour maps of the land surface, bottom of the Tiva Canyon hydrogeological unit (TCw), and isopach maps of the Paintbrush and Topopah Spring units (PTn and TSw, respectively). It specified fault alignments and offsets using information from the USGS. The USGS collaborated in the development of this model by providing input and reviewing the resulting maps.

Concurrent with the Wittwer et al. work, the USGS developed a geological model (Buesch et al., 1995) of the proposed repository area using the LYNX modeling software package. This required a detailed study of fault alignments and offsets and the structure of the subsurface geology at Yucca Mountain. The result

Geological Model Development and Vertical Layering Scheme for the Numerical Grid

was a flexible model with numerous layers that could be used to develop standardized numerical grids at Yucca Mountain. The model also included a surface representing the distance to the top of a zone of prevalent zeolites from the bottom of the Topopah Spring basal vitrophyre.

Recent development of a standardized 3-D geological framework model has been performed by the Yucca Mountain Management and Operating Contractor (M&O) staff. Zelinski and Clayton (1996) have created a 3-D model which includes 2-D fault planes and fault offsets over an extended area centered on the proposed repository. The fault map used in this model is based on preliminary work by Day et al. (1996). This recent work shows more major faults (defined as having offsets greater than 10 meters) and structural complexities in the unsaturated zone than have been previously shown. The 3-D model includes explicit layers for many of the geological formations found in the unsaturated zone. Future versions of the model will include 3-D faults and zones of alteration. It is intended that this model will be used by all of the participants in the Yucca Mountain Project to generate numerical grids. However, the 3-D geological framework model was only in preliminary stages of development at the time that numerical grids were required for the UZ model work during FY96. Therefore, a geological model for use in developing numerical grids was prepared. This model built on the models developed by the USGS (Buesch et al. 1995) and Wittwer et al. (1992) using available new data. The work included selecting the important layers for inclusion into the geologic model and creating contour maps of the important surfaces.

This chapter presents the results of an evaluation of these previous models and available hydrogeologic data. The evaluation resulted in a selection of the vertical layers which are important to subsurface flow processes and these layers have been included in the numerical grid of the site-scale UZ model described in Chapter 5 (Haukwa et al., 1996). The chapter also presents some of the contour and isopach maps of the geological formations which were used to create the numerical grids used in the modeling studies described in this report. It also describes the rationale behind the extension of the site-scale model boundaries.

2.1.1 QA status of data and software used in this chapter

The development of a geological model of the unsaturated zone at Yucca Mountain is based on many data sources. The most important data sources are the boreholes logs with formational descriptions and layer depths. Secondary sources include pavement studies, section measurements, and geophysical logging and core sample property measurements.

The implementation of a Quality Assurance programs in recent years by participants on the Yucca Mountain Project means that many of the data collected recently are designated Q. However, much of the previous work is not Q, especially in areas away from the proposed repository block. It is imperative that these non-Q data be used in any development of a geological model charac-

terizing areas away from the proposed repository. Therefore, the resulting maps and numerical grids in these areas cannot be considered Q. However, in the vicinity of the proposed repository area, there are sufficient data from Q sources that numeric grids for this area can be considered Q, with any non-Q data being used to only corroborate the Q sources. A complete listing of Q and non-Q data sources used in the development of the geological model is provided in the references.

The work done to create these maps for the geologic model has been documented in the Yucca Mountain Project Scientific Notebook YMP-LBNL-GSB-1.5, which is a subnotebook of the Scientific Notebook for the UZ Model.

2.2 *Extended Model Domain*

The boundaries for the site-scale model were originally chosen to coincide with the alignments of known or suspected faults (Wittwer et al., 1995). The eastern and western boundaries were fixed by the traces of the Bow Ridge and Solitario Canyon faults, respectively. The northern boundary roughly follows the alignment of the proposed Yucca Wash fault shown in the Scott and Bonk Geological Map of Yucca Mountain (1984). In the absence of a major east/west fault to the south of Yucca Mountain, the boundary was chosen to be far enough away from the proposed repository area so that it would not significantly affect the model simulation results. The lower horizontal boundary for the model was established by assuming a relatively flat water table across the entire model domain.

The decision to use major faults as the model boundaries was re-evaluated because the results of some modeling studies (Ahlers et al., 1995; Wittwer et al., 1995) suggest that the major faults may serve as fast pathways to flows of moisture and vapor within Yucca Mountain. Current repository designs have the western limit of the proposed drifts relatively close to the western boundary of the site-scale model as shown in Wittwer et al. (1995). This proximity to the model boundary certainly affects the thermal gradient and transport processes studied during simulations with the UZ model.

Furthermore, extensive measurements of water-table altitudes in boreholes have verified the rise of more than 300 meters in the potentiometric surface from the proposed repository vicinity to near Yucca Wash, and a rise of about 40 meters from the repository to boreholes on the western side of the Solitario Canyon fault. There are some indications that the apparent gradient measured near Yucca Wash may be due to perched water (J. Czarnecki, USGS, personal communication, April, 1995), and the perched water bodies could be recharged from the watershed area north of Yucca Wash. Spatially variable precipitation patterns (Hevesi et al. 1994) for various storms show a general increase in precipitation amounts to the northwest of the proposed repository area. This increase

Geological Model Development and Vertical Layering Scheme for the Numerical Grid

is also reflected in spatially variable net infiltration maps recently generated by the project (Flint et al., 1996, in prep.) This increased infiltration could be associated with the measured perched water bodies. Based on this, the northern limit of the model could potentially include the recharge area of the increased infiltration up to the watershed boundary located near Chocolate Mountain.

Therefore, to avoid significant boundary-condition effects on the simulations, to allow studies of the effects of the major faults, and to be able incorporate the perched water bodies and significant recharge areas observed at Yucca Mountain, the model boundaries have been extended in all directions. The extension is intended to cover the entire area which may be required for study in future simulations. Since various studies of the UZ require different grids, the entire extended area does not have to be covered by each grid that is generated.

A plan view of the maximum extended grid which may be required for future site-scale studies based on present information is shown in Figure 2.2-1. The figure also shows the original model boundary (Wittwer et al., 1992), the proposed repository outline, and the controlled area boundary, as well as the locations of representative boreholes in the vicinity of Yucca Mountain.

Figure 2.2-1
Extended Model and Project Boundaries. Locations of boreholes greater than 100 meters in depth providing geologic control are also shown.

Figure 2.2-1 shows that most of the boreholes that provide geological control for the model are located within the original model boundaries. Therefore, the geological control provided by boreholes for the extended model region is minimal, especially in the area north of Yucca Wash. The small number of boreholes located adjacent to major faults does not provide good control on the magnitude of layer offsets across the faults, an important feature for the 3-D extended model.

2.3 Vertical Layer Subdivision

Montazer and Wilson (1984) developed a conceptual model which divided the subsurface geological formations at Yucca Mountain into five main hydrogeological units based on the degree of welding found in the formations. The units consist of moderately to densely welded tuff zones alternating with zones of non- to partially welded ash flow tuffs and bedded air fall tuffs. The units include:

1. The Tiva Canyon Welded (TCw) Unit consisting of the moderately to densely welded portions of the Tiva Canyon Tuff of the Paintbrush Group.
2. The Paintbrush Nonwelded (PTn) Unit consisting of the partially- to non-welded portions of the Tiva Canyon Tuff underlying the TCw, alternating layers of bedded tuffs and the Yucca Mountain and Pah Canyon tuffs, and the non- to partially welded portions of the upper Topopah Spring Tuff.
3. The Topopah Spring Welded (TSw) Unit consisting of the moderately to densely welded portions of the Topopah Spring Tuff down to and including the densely welded basal vitrophyre.
4. The Calico Hills Nonwelded (CHn) Unit consisting of the formations underlying the basal vitrophyre of the Topopah Spring Tuff down to the water table. These formations include the following: A) moderately to non-welded portions of the lower Topopah Spring Tuff; B) the Calico Hills Formation and underlying tuffaceous beds; C) the Prow Pass Tuff of the Crater Flat Group and the underlying tuffaceous bed; and D) the non- to partially welded portion of the upper Bullfrog Tuff of the Crater Flat Group.
5. The Crater Flat Undifferentiated (CFu) Unit, consisting of the lower Bullfrog and Tram Tuffs of the Crater Flat Group, and the interbedded tuffs.

The first four units are the ones commonly found in the unsaturated zone in the vicinity of the proposed repository block. The fifth unit is only found above the water table in limited areas beneath Yucca Crest to the south of the proposed repository area. Table 2.2-1 shows the relationships between the geological formations and the hydrogeological units, as well as the Buesch et al. (1995) and

Geological Model Development and Vertical Layering Scheme for the Numerical Grid

Moyer and Geslin (1995) zonations for the geological formations. It also presents the UZ model layer names used in the vertical layering scheme which will be presented below.

Table 2.2-1 Relationship between Model Hydrogeological Units and Geological Formations			
Geological Unit	Welding Intensity/ Formation Name (Buesch et al., 1995)	Model Layer Name	Hydrogeological Unit
PAINTBRUSH GROUP			
Tiva Canyon Tuff	M,D ¹ (Tpcxxx)	tcw11 tsw12	Tiva Canyon (TCw)
	D- Basal Vitrophyre (Tpcpv3) M (Tpcpv2)	tcw13	
	N,P (Tpcpv1)	ptn21	
Bedded tuff	N (Tpbt4)		Paintbrush (PTn)
Yucca Mountain Tuff	N,P,M (Tpy)	ptn22	
Bedded tuff	N (Tpbt3)	ptn23	
Pah Canyon Tuff	N,P,M (Tpy)	ptn24	
Bedded tuff	N (Tpbt2)	ptn25	
Topopah Spring Tuff	N,P (Tpdrv3)		Topopah Spring (TSw)
	M (Tpdrv2)	tsw31	
	D -Upper vitrophyre (Tpdrv1)		
	M,D (Tpdrv)	tsw32	
	M,D,L (Tpdrv)		
	M,D,L (Tpdrv)	tsw33	
	D (Tpdrv)	tsw34	
	M,D,L (Tpdrv)	tsw35	
	D (Tpdrv)	tsw36	
	D (Tpdrv)	tsw37	

Geological Model Development and Vertical Layering Scheme for the Numerical Grid

Table 2.2-1 (cont.) Relationship between Model Hydrogeological Units and Geological Formations			
Geological Unit	Welding Intensity/ Formation Name (Buesch et al., 1995)	Model Layer Name	Hydrogeological Unit
Bedded tuff	N,P,M; may be altered (Tptpv1, Tptpv2) N; may be altered (Tpbt1)	ch1 (vc or zc)	Calico Hills (CHn)
Calico Hills Formation	N; unaltered (Ta - Vitric)	ch2vc	
	N; altered (Ta - Zeolitic)	ch3zc	
	N; may be altered (Thbt)	ch4 (vc or zc)	
CRATER FLAT GROUP			
Prow Pass Tuff	N; may be altered (Tpc) Unit 4 ³		
	P,M Unit 3	pp3vp	
	N,P; generally altered Units 2,1	pp2zp	
Bedded tuff	N; generally altered (Tpcb1)		
Upper Bullfrog Tuff	N,P; generally altered (Tcb)		
Middle Bullfrog Tuff	P,M	bf3vp	
Lower Bullfrog Tuff	N,P; generally altered	bf2zp	Crater Flat Undifferentiated (CFu)
Bedded tuff	N; generally altered (Tcbt)		
Upper Tram Tuff	N,P; generally altered (Tct)		

1 Welding Intensity N=Non-; P=Partially; M=Moderately; D=Densely

2 L=Lithophysal Zone

3 Units per Moyer and Geslin (1995)

The original site-scale model grid described in Wittwer et al. (1995) was prepared by subdividing the main hydrogeological units (TCw, PTn, TSw, CHn) into 17 sublayers to represent hydrogeological variations in the subsurface. This includes the representation of significant layer offsets due to faults and the dipping of strata observed at Yucca Mountain. The selection of the vertical layering of the model is summarized below.

1. A review was done of the available logs to determine the elevations of the contacts between the major units.
2. The contact data was used to determine the elevation of the base of the TCw, including offsets due to faults, and thicknesses of the other major units.
3. An elevation contour map for the base of the TCw, isopach maps for the other major units, and a water table contour map were developed based on the borehole log information. A topographic map of the land surface elevation was obtained.

Geological Model Development and Vertical Layering Scheme for the Numerical Grid

4. The maps were used to develop the main unit thicknesses at each node point of the horizontal model grid.
5. For modeling purposes, the main units were divided into sublayers to provide for thin boundary layers at the unit contacts and thicker sublayers in the center of the units. The thin boundary layers allowed the resolution of possible strong gradients in driving forces between the units during simulations, thus minimizing grid discretization errors. The subdivision of the units was performed according to a simple set of rules developed to provide thin boundary layers. The thickest units were given the greatest number of sublayers to reduce the thicknesses of the sublayers in the model grid. The relatively thin TCw and PTn were each given three sublayers, the TSw was assigned 6 sublayers, and the CHn was given a total of 5 sublayers. After subdivision, the sublayers were assigned rock and fracture properties from laboratory measurements of permeabilities and characteristic curves for the various formations in the geological members. The values were assigned to the sublayers based on a rough vertical association of model sublayers to geological formations.

As a result of the procedures to develop the original model vertical layers and the assignment of hydrogeological properties to them, the following issues were identified:

1. The top layer between the land surface and the bottom of the TCw was assumed to consist entirely of TCw. This assumption was valid except in the alluvial washes and small regions where the nonwelded Rainier Mesa Formation overlies the Tiva Canyon Tuff. In these areas, the gridding procedure led to an overestimate of the thickness of the TCw. Significant alluvial deposits can also be found on the downthrown side of the major faults.
2. The rules for subdivision used in creating the sublayers led to a grid with sublayer boundaries that only roughly corresponded to the physical location of geologic layer boundaries observed in boreholes at Yucca Mountain. Therefore, model runs to simulate observed borehole data could only roughly match the measurements since the sublayer node points in the numerical grid did not correspond well to the geological formation mid-point elevations.
3. The TCw was divided into three sublayers. Since upper portions of the TCw are often missing due to erosion, the top two model layers could not be consistently correlated with explicit geologic formations across the model domain. However, the original model layers were assigned these layers rock properties from these explicit geologic layers.
4. Due to the dipping geological beds and offset layers from faulting, the relatively flat water table used to define the bottom boundary of the original

site-scale model intercepted a number of different geological formations, which included the bottom of the geological formations of the Topopah Spring Tuff down to the Bullfrog Tuff of the Crater Flat Group. However, the subdivision process used to create the Calico Hills vertical grid subtracted the elevation of water table from the elevation of the base of the TSw and then partitioned that result into five layers. The bottom two layers were assigned zeolitic properties. This did not provide an accurate representation of the formations intercepted by the water table or the presence of zeolitic alteration as it occurs in the CHn.

In order to address some of the above issues, an evaluation of available data was undertaken before a revised vertical layering scheme for the UZ model was selected. The evaluations included reviews of the results of grid discretization studies, available borehole data such as saturation, water-potential, porosity, and gas pressure measurements, and reports on the geological formations at Yucca Mountain characterizing lateral continuity and alteration. The results of the evaluations as discussed in the following sections guided the selection of vertical layers in the new grids for the UZ model.

**2.3.1
Gas pressure measurements
and modeling results**

The results of gas flow analyses and simulations performed with the pneumatic pressure data gathered by J. Rousseau of the USGS were presented in Ahlers et al. (1995). The results of the analyses and modeling showed that most of the attenuation of the pneumatic signal measured in boreholes USW NRG-7/7a and -NRG-6 occurred across the bedded tuff layer (Tpbt3) separating the Yucca Mountain and Pah Canyon Tuffs in the PTn. Some attenuation, however, did occur across the densely welded basal vitrophyre and the underlying moderately welded and sometimes highly altered formation serving as the bottom two layers in the TCw. The fact that little attenuation occurred elsewhere in the TCw indicated that there are numerous well-connected fractures in the formations above the basal vitrophyre. Although a relatively good match of observed gas pressures and predicted pressures was achieved by Ahlers et al. (1995) using three sublayers to characterize the PTn, a better fit occurred when five sublayers were used in the model corresponding to the main geologic formations in the PTn.

**2.3.2
Borehole data
measurements**

Numerous laboratory measurements have been performed on core samples from boreholes at Yucca Mountain. Figures 2.3.2-1 and -2 present the results of the core sample measurements of porosity, saturation, and capillary pressure for borehole SD-9, which is representative of hydrogeologic conditions found in the other boreholes. The data show that the welded hydrogeological units have generally higher saturations and potentials and lower porosities than the mostly nonwelded units such as the PTn and the CHn. Saturations can be higher than 90 percent in some of the densely welded formations in the TCw and TSw, while they can be as low as 30% in the PTn and 60% in the CHn. If a significant portion of the CHn in SD-9 was vitric as is found in other boreholes,

Geological Model Development and Vertical Layering Scheme for the Numerical Grid

the saturation in the vitric portion at the top few meters might have been as low as 20 percent. Because most of the unit is altered, however, the saturations are high. In general, as the porosity increases (nonwelded units), the saturation decreases because the pores get larger and can retain less water due to smaller capillary suction.

Figure 2.3.2-1.

Core Sample Porosity and Saturations Measurements for Borehole SD-9. Q data measured by L. Flint, USGS; DTN 950308312231.004. Data averaged with a sliding mean of 5 points. Thick solid line is saturation. Solid line is porosity. Horizontal solid lines show hydrogeological unit boundaries. Dashed lines show geological layer boundaries.

Geological Model Development and Vertical Layering Scheme for the Numerical Grid

Figure 2.3.2-2.
Core Sample Capillary Pressure Measurements for Borehole SD-9. Q data measured by L. Flint, USGS; DTN 950308312231.004. Data averaged with a sliding mean of 5 points. Heavy solid lines show hydrogeological unit boundaries. Dashed lines show geological layer boundaries.

The saturations in the PTn are relatively low. The boundaries where the PTn grades into the densely welded TCw and TSw show high saturations. This behavior is also seen in the middle portion of the Tpy (Yucca Mountain Tuff) which shows a decrease in porosity and an increase in saturation. The middle portion of the Tpy is slightly more welded than the rest of the formation. Capillary pressures are near 0 bars in the PTn sublayers.

The relatively thick tuff units which comprise the TSw show variations in saturation and water potential across each layer. The data indicate that layer boundaries are not distinct but are gradational. Porosities, saturations and potentials for each formation vary distinctly due to geological heterogeneities. The Tptm and Tptpl (zonation by Buesch, et al., 1995) layers underlying the upper vitrophyre show a relatively consistent increase in saturation over the interval from a low of about 40% at the PTn/TSw interface, to a high nearing 90% at the Tptpmn (middle nonlithophysal) boundary.

In the underlying Tptpmn, Tptpl (lower lithophysal), and Tptpln (lower nonlithophysal) formations, average saturations are higher for the nonlithophysal layers than for the lithophysal layers. The lithophysal cavities will cause

some differences in flows processes when compared to the nonlithophysal layers. The basal vitrophyre is evident from a distinct decrease in porosity, but the effect on saturation seems to be dominated by the presence of the less welded underlying layers with increased porosities and decreased saturations. The underlying layers consist of the moderately to non-welded Topopah Spring and a bedded tuff. The topmost of these layers is mostly vitric, which explains the drop in saturations.

In the rest of the CHn, however, there is a high degree of zeolitic alteration, which does not affect porosity significantly but increases the saturations and capillary pressures. This is why saturations are above 90% except in some localized areas and why potentials are similar to those measured in welded portions of the TSw. The potentiometric surface elevation is about 730 meters above sea leve (masl) in the vicinity of SD-9, which is close to the top of the Prow Pass (Tcp) Unit 3. This unit is generally described as partially to moderately welded and devitrified, which prevented it from being significantly altered after deposition. Where a significant portion of this unit is above the water table, matrix saturations are observed to drop significantly, as in UZ#16 (Q Borehole Data from L. Flint, USGS, 1996. DTN GS940508312231.006).

Other data which were reviewed include borehole logs which report the contact depth of geological formations, zones of alteration, degree of welding, and fracture frequency. This provided information about the average layer thickness, degree of welding, presence of lithophysal cavities, and other data which affect flow processes in the UZ. The references sections presents a summary of the data sources used in this review.

The results of geophysical logging of the boreholes were also reviewed. Nelson (1996) has prepared non-Q saturation estimates for 25 boreholes at Yucca Mountain based on geophysical logging results (Nelson et al., 1989; Muller and Kibler, 1985). The evaluation included an identification of possible zeolitic zones. These data were compared to borehole log reports of zones of alteration to corroborate the thicknesses of zeolitic layers for use in the UZ model.

2.3.3 Report Evaluation

The report evaluation included the review of the geological model reports discussed in the introduction section of this chapter. In general, as data have become available from borehole and geology studies of Yucca Mountain, the models have become more complex with more layers. The reports described below are examples of the types of detailed studies that have been conducted at Yucca Mountain.

Moyer et al. (1995) reported the results of a study of the PTn. They examined borehole core samples, evaluated available laboratory data, and used the results to divide the PTn into numerous sublayers. Isopach maps showed that the Yucca Mountain and Pah Canyon Tuffs, as well as the bedded tuff found

between them, pinch out in the vicinity of the proposed repository area. They also noted that the Pah Canyon and Yucca Mountain Tuffs have significant partial to moderately-welded zones in the northern portion of the extended model which may affect flow patterns in the unsaturated zone there. Preliminary modeling runs evaluating the unsaturated zone showed that the PTn sublayers could cause lateral diversion of infiltrating moisture related to the variations in hydrogeological properties between adjacent sublayers and sublayer thicknesses.

Moyer and Geslin (1995) reported the results of their study of the CHn which underlies the Topopah Spring basal vitrophyre. They published isopach maps of the various sublayers in their analysis, and provided a discussion of zones of alteration and zeolites. They concluded that there is not a consistent surface in the Calico Hills Formation that serves as the contact of the vitric and zeolitic layers. The formation varies locally: 1) an area in the vicinity of the proposed repository with no alteration in the Calico Hills Formation; 2) an area to the northeast of the proposed repository consisting of interbedded vitric lavas and zeolitic tuffs; and 3) the remainder of their area of study consisting wholly of zeolitic tuffs or some vitric tuffs underlain by zeolitic tuffs.

Robinson et al. (1995) presented a draft report containing the results of an analysis of borehole and mineralogic data to define zeolitic layers below the TSw. Their analysis presented two cases, one of which defined zeolitic layers based on the available data (nominal case), and one of which defined a maximal zeolitic layer thickness in each hole. They then used these data to develop grids which were used in transport modeling studies.

Flint (1996, in prep.) is conducting an independent analysis that will present matrix rock properties for the formations which are considered important for subsurface flow processes. A review of preliminary tables from this report shows that properties are presented for all of the layers discussed in the analysis of the SD-9 borehole data.

This report also continued an approach of developing correlations between rock porosity and hydrogeologic properties. One of the early proposals of this approach was from Montazer and Wilson (1984) who showed that there were distinct porosity differences between the non-welded and welded units. Indeed, this variation served as the basis for their hydrogeologic unit delineation. They stated that the welding process generally results in small matrix porosity and small pore sizes; thus, matrix permeability is less in the welded units than in the nonwelded units.

The approach was continued by Flint et al. (1996b) in analyzing the results of measurements of permeabilities and van Genuchten model fitting parameters on outcrop samples. The correlations between porosity and permeability

were better statistically than those between porosity and the van Genuchten parameters.

Based on the report evaluation, geologic layers were identified which should be explicitly represented in the model grid on the basis of porosity and hydrogeologic parameters. The reports showed that the geological formations can vary in thicknesses and welding across the model domain, which means that their effects on UZ flow processes are also variable. The variable hydrogeologic parameters can be characterized with regression equations presented in the reports. Important altered zones in the CHn were identified from these reports for inclusion into the UZ model.

2.3.4 Grid Discretization Studies

The results of the grid discretization studies performed on a 2-D cross-section submodel of the UZ model are described in detail in Chapter 5 (Haukwa et al., 1996). In summary, the study concluded that the greatest increase in computational precision occurred when the grid was refined by doubling the number of layers. In particular, the top layers of the TSw were identified as important areas for grid refinement because of the variations in permeability between the less welded formations overlying the more densely welded formations.

This review and the others described in Sections 2.3.1 through 2.3.3 were done to address some of the issues identified from the preparation of the numerical grid for the UZ model described in Wittwer et al. (1995). The results of the evaluation guided the selection of vertical layers for inclusion in the new grids for the UZ model. The reviews indicated that the layering could be refined to include hydrogeologically and computationally important layers which had previously been represented by composite layers. Altered zones could be explicitly represented in the model, and variations in hydrogeologic parameters could be characterized through regression equations.

2.4 Sublayer Selections

The selection of vertical sublayering for the site-scale model was done based on the reviews of the data and analyses. Variations in measured hydrologic properties and in porosities which correlate to hydrologic properties for various formations were used to define important sublayers. Other sublayers were chosen because existing studies indicated that they were important for flow.

Another criterion in the selection process included selecting relatively thin sublayers consisting of geological formations at the boundaries between non-welded and welded hydrogeological units. This was done in order to resolve possible strong gradients in driving forces occurring during modeling. In some cases, relatively thin adjacent layers with similar hydrologic properties were

Geological Model Development and Vertical Layering Scheme for the Numerical Grid

combined into one model layer as shown in Table 2.2-1. This was done to prevent the thicknesses of adjacent model layers from varying too rapidly in the model grid and to prevent grid aspect ratio problems. These two criteria were used to minimize grid discretization errors.

Once the sublayer selections were made, isopach and structure contour maps were developed for the main hydrogeologic units and important sublayers such as the PTn geologic formations and altered zones in the CHn. These maps extend across the maximum area which might be used in modeling studies in the future. They do not, however reflect areas where layers may be missing or absent due to erosion (such as in washes). This is accounted for during the numerical gridding by comparing the predicted elevation of a layer midpoint to topographic elevation information. If the land surface elevation is less than the predicted layer midpoint elevation, this layer is omitted from the numerical grid.

Although most of the maps have contours north of Yucca Wash, it is important to understand that the area north of Yucca Wash is very different, geologically speaking, than the region near the proposed repository. There are numerous faults and additional geological formations not present at Yucca Mountain. Therefore, the maps are drawn to be able to provide continuous model layers during gridding, but it is understood that any nodes in this area would need to be given different hydrogeological properties to account for the geological differences. Exactly what those properties might be has not yet been studied in detail by the project as there are few boreholes located in that area.

2.4.1 TCw Sublayers

The TCw in the UZ model is represented with three sublayers. The bottom sublayer (tcw13) corresponds to the basal vitrophyre (Tpcpv3) and moderately welded portion (Tpcpv2) of the Tiva Canyon Tuff. These two layers are found at a transition zone from many to few fractures, and have been reported to be altered, especially the Tpcpv2, providing a barrier to flow (L. Flint, USGS, Personal Communication, October 1995). Neither the Tpcpv3 nor the Tpcpv2 is laterally continuous across the entire Yucca Mountain area based on borehole log data, but the combined thickness of the two layers averages about 6 meters. This sublayer provides a thin boundary layer for the model to resolve possible strong hydraulic gradients in driving forces occurring during simulations. A contour map of the base of the TCw developed for the extended model is presented in Figure 2.4.1-1.

Geological Model Development and Vertical Layering Scheme for the Numerical Grid

Figure 2.4.1-1

Tiva Canyon Hydrogeological Unit Bottom Elevation Contour Map. Elevation contours in meters. Fault alignments as shown in 3-D Geological Framework Model (Zelinski and Clayton, 1996). Circles indicate borehole locations used for geological control. UZ model boundary incorporating Solitario Canyon fault and G-2 perched water body is shown.

The TCw has been partially or entirely removed from the mountain by erosion, especially in washes. Because portions of the TCw are absent across the mountain, it is difficult to choose specific formations to explicitly use as the remaining sublayers in the model. Therefore, the remaining two sublayers (tcw11 and tcw12) were determined by equally dividing the total thickness of the overlying Tiva Canyon not removed by erosion.

A contour map showing the depth of alluvium in washes and valleys at the site was developed based on borehole data and maps from the GIS database showing the contact between the bedrock and alluvium. This map was used to establish the top of the TCw in washes and valleys with significant deposits of alluvium.

2.4.2 PTn Sublayers

The PTn in the UZ model consists of five sublayers based on the pneumatic data analysis discussed in Section 2.3.1. The top sublayer (ptn21) combines the formations of the partially- to nonwelded Tiva Canyon Tuff (Tpcpv1) and the underlying bedded tuff (Tpbt4) where present. The underlying sublayers ptn22, ptn23, and ptn24 consist of the Yucca Mountain (Tpy), interbedded tuff (Tpbt3), and Pah Canyon (Tpp) Tuffs where present, respectively. Sublayer ptn25 consists of the bedded tuff underlying the Pah Canyon Tuff and the non- to partially-welded portion of the Topopah Spring Tuff. Sublayers ptn22, ptn23, and ptn24 pinch out in the vicinity of the proposed repository area. The isopach map of the entire PTn developed for the extended model is presented in Figure 2.4.2-2. This map agrees well with the map developed for the 3-D geological framework model by Zelinski and Clayton (1996). Individual isopach maps have also been developed for the sublayers so their lateral variations and pinch-outs can be characterized properly in the model gridding effort. One of these isopach maps for the Yucca Mountain Tuff is shown as an example in Figure 2.4.2-3.

Figure 2.4.2-1
PTn Isopach Contour Map. Thickness in meters. Circles indicate borehole locations used for geological control. Squares indicate locations of measured outcrop sections from Moyer and Geslin (1995).

Figure 2.4.2-2

Yucca Mountain Tuff Isopach Map. Thickness in meters. Circles indicate borehole locations used for geological control. Squares indicate locations of measured outcrop sections from Moyer and Geslin (1995).

2.4.3 TSw Sublayers

The TSw in the extended model consists of seven sublayers. The subdivision was chosen based on variations of porosity, presence of lithophysal cavities, fracture frequency, and saturation and capillary pressure variations. The top sublayer, tsw31, corresponds to the moderately welded and upper vitrophyre formations (Tptrv2 and Tptrv3, respectively) at the top of the Topopah Spring Tuff. The bottom sublayer, tsw37, consists of the densely welded basal vitrophyre near the base of the Topopah Spring Tuff. Sublayers tsw32 through tsw36 correspond to the major geologic layers encountered between the upper and lower vitrophyres (Tptm, Tptpul, Tptpmn, Tptpll, and Tptpln, respectively).

Based on the results of the grid discretization studies, sublayers tsw32 and tsw33 should be subdivided into additional computational layers to add the refinement necessary to minimize grid effects. The isopach map developed for the entire TSw is presented in Figure 2.4.3-1. This map agrees well with maps developed for the TSw by Zelinski and Clayton (1996) in the 3-D Geological

Framework Model and by Wittwer et al. (1995) for the original site-scale UZ model.

Figure 2.4.3-1.
TSw Isopach Contour Map. Thickness in meters. Circles indicate borehole locations used for geologic control.

2.4.4 CHn and CFu Sublayers

The basis for subdivision within the CFu and CHn is the degree of alteration. Alteration of vitric tuffs can occur when they are exposed to heat and water. Furthermore, alteration to clays is a slow but on-going process at the mountain, with smectite commonly found in core samples. Based on the alteration zones, the CHn and CFu in the extended model consist of nine sublayers. The upper sublayer ch1vc combines the moderately to nonwelded portions of the Topopah Spring Tuff underlying the basal vitrophyre and the bedded tuff that overlies the Calico Hills Formation. In places the layer is altered and is

referred to as sublayer ch1zc. Sublayers ch2vc and ch3zc represent the vitric and zeolitic portions of the Calico Hills Formation where present. Over most of the model area, the total thickness of the Calico Hills Formation is altered. However, in an important area near the southern proposed repository area, the Calico Hills formation is unaltered.

Sublayer ch4zc corresponds to the bedded tuff underlying the Calico Hills Formation (Thbt) and Unit 4 (Moyer and Geslin, 1995) of the Prow Pass. Both of these layers are found to be altered at Yucca Mountain. However, maps of the extent of alteration (Moyer and Geslin, 1995) for the layers show that the alteration boundary of the Thbt layer incorporates the alteration zone for the Prow Pass Unit 4. Therefore, the alteration boundary for Thbt was used to define the altered zone of the ch4zc for modeling purposes. Where the Thbt is not altered, it is referred to as sublayer ch4vc.

Sublayer pp3vp corresponds to the variably welded and devitrified Unit 3 of the Prow Pass underlying Unit 4. The devitrification and welding has prevented this unit from undergoing significant alteration. Sublayer pp2zp consists of a composite of Units 1 and 2 of the Prow Pass, the lower Prow Pass bedded tuff, and the non-welded portion of the upper Bullfrog. These layers are generally reported to be altered in borehole logs and by mineralogic studies, so the entire layer is considered to be altered across the model domain.

The next layers repeat the pattern of the pp3vp and pp2zp. Sublayer bf3vp consists of a variably welded and somewhat devitrified middle portion of the Bullfrog which is mostly unaltered. Sublayer bf2zp consists of a composite of lower Bullfrog, the lower Bullfrog bedded tuff, and the non-welded portion of the upper Tram. Sublayer tr3zp consists of any portion of the Tram still in the unsaturated zone. This layer is reported to be significantly altered in the boreholes deep enough to penetrate it.

Due to the dipping of the strata and layer offsets caused by major faults, the water table intercepts each of the formations of the CHn and CFu, and even the lower TSw, at different locations in the model area. To account for this, individual isopach maps were developed for the various sublayers. A sample isopach map combining sublayers ch2vc and ch3zc (representing the combined vitric and zeolitic portions of the Calico Hills geological formation) is presented in Figure 2.4.4-1. This map agrees well with a map covering the central portion of the extended model area presented by Moyer and Geslin (1995).

Geological Model Development and Vertical Layering Scheme for the Numerical Grid

Figure 2.4.4-1
Calico Hills Formation Isopach Map. Thickness in meters. Circles indicate locations of boreholes used for geological control.

2.4.5 Water Table

Two contour maps of the water table were developed. The first map was developed assuming that the potentiometric surface measured at boreholes WT-6 and G-2 is a perched water body and the true water table is relatively flat over the model area. This map provides a larger volume for the UZ model and allows the simulation of perched water bodies above the regional water table. However, the water table is assumed to rise across the Solitario Canyon fault to match the elevations measured in H-6 and WT-17. In this case, the Solitario Canyon fault is assumed to act as a flow barrier. This map is similar to the one presented in Wittwer et al. (1995) with the exception of the rise in potentiometric surface elevation west of the Solitario Canyon Fault. this rise is assumed to occur as a step across the fault, with the fault acting as a flow barrier.

Geological Model Development and Vertical Layering Scheme for the Numerical Grid

The second map assumes that the potentiometric surface measurements in the boreholes reflect the true water table and incorporates the moderate and steep gradients reported in the Solitario Canyon and Yucca Wash regions of the study area. The Solitario Canyon fault is also assumed to act as a flow barrier in this map with the rise in water table occurring across the fault zone. This map is presented in Figure 2.3.6. The map agrees well with a draft water table map covering the extended model area south of Yucca Wash prepared by Tucci and Burkhardt (1995).

Recent pump testing of borehole G-2 by the USGS indicates that the potentiometric surface measured in G-2 may indeed be from a perched water body (J. Sass, USGS, personal communication, August 1996). Therefore, the grids developed for the UZ model used the first map similar to that shown in the Wittwer et al. (1995) report. This provides a grid which can be used to simulate the locations and variations in perched water bodies reported at Yucca Mountain as described in Chapter 7 (Wu et al., 1996).

Figure 2.4.5-1

Water Table Map. Map assumes borehole measurements reflect water table elevation from an unconfined aquifer. Dotted lines indicate potentiometric surface contours from Ervin et al. (1995). Circles indicate borehole locations used for potentiometric surface control.

2.5 Summary and Conclusions

**2.5.1
Summary**

The original boundaries of the site-scale model as presented in Wittwer et al. (1995) were chosen to coincide with major faults bounding an area relatively well-characterized by existing borehole information and hydrogeological studies. However, the results of preliminary modeling simulations described in that report showed that the presence of faults can have significant impacts on flow patterns at Yucca Mountain. The assumptions used for boundary conditions also affect the simulation results near the boundaries. To address these issues, boundaries have been chosen that define the maximum area of interest for the site-scale model based on known information about the site. These boundaries incorporate a large area; however, grids for the site-scale model may be developed for only a portion of the area depending on the required scale of the model study.

Numerical grids were required as part of FY96 work for portions of the extended area, and the 3-D geologic framework model was not available until late FY96. Therefore, a geological model of Yucca Mountain was prepared to use in extending the various grids as part of the UZ modeling effort. As part of geologic model preparation, the vertical sublayering scheme used in the original site-scale model was evaluated. The evaluation included a review of existing borehole data measurements, available reports, and grid-discretization studies. The geologic model consists of elevation contour and isopach maps for the important model layers which are used in the gridding.

**2.5.2
Conclusions**

The conclusions of the boundary extension and vertical layering selection process include the following:

- The layering scheme was improved by refining the layers to explicitly include more of the important hydrogeologic layers. Model studies using pneumatic data and evaluating lateral diversion of flow indicate that these layers include the Yucca Mountain and Pah Canyon Tuffs and an interbedded unit.
- Grid discretization studies indicated that grid effects could be minimized by refining the grid for the layers at the top of the TSw.

Due to the non-Q status of the borehole logs used for geologic control in the extended model areas, the geologic model is not Q over its entire domain. However, enough Q logs exist in the vicinity of the potential repository block to consider the central block of the model Q. The above conclusions pertaining to the central block area are also Q.

**2.5.2
Future Work**

Data from additional studies will become available as the project continues. These include geophysical and mineralogical data defining zones of alteration. The 3-D geologic framework model by Zelinski and Clayton (1996) should pro-

vide standardized geological layering and fault geometries for future numerical grids. However, it does not yet contain information about altered zones which are critical for flow and transport models. If these and other important unsaturated zone aspects are not incorporated into the geologic framework model, LBNL will continue to revise the model described in this report to reflect the latest available information for use in preparing numerical grids for the site-scale model.

2.6 *References*

- Ahlers, C.F., T.M. Bandurraga, G.S. Bodvarsson, G. Chen, S. Finsterle, and Y.S. Wu, Performance analysis of the LBNL/USGS three-dimensional unsaturated zone site-scale model, Lawrence Berkeley National Laboratory, 1995a.
ACCN: MOL.19960208.0091-0097
DTN:LB092995312293.001 (Non-Q)
- Ahlers, C.F., T.M. Bandurraga, G.S. Bodvarsson, G. Chen, S. Finsterle, and Y.S. Wu, Summary of model calibration and sensitivity studies using the LBNL/USGS three-dimensional unsaturated zone site-scale model, Lawrence Berkeley National Laboratory, 1995b.
- Buesch, D.C., R.W. Spengler, T. C. Moyer, and J.K. Geslin, Revised stratigraphic nomenclature and macroscopic identification of lithostratigraphic units of the Paintbrush Group exposed at Yucca Mountain, Nevada, U.S. Geological Survey Report OFR 94-469, U.S. Geological Survey, 1995.
- Day, W.C., C.H. Potter, D.S. Sweetkind, and R.P. Dickerson, Preliminary bedrock geological map of the Central Block Area, Yucca Mountain, Nevada, April 26, 1996.
- Ervin, E.M., R.R. Luckey, and D.J. Burkhardt, Revised potentiometric-surface map, Yucca Mountain and vicinity, Nevada, U.S. Geological Survey WRI-93-4000, U.S. Geological Survey, 1995.
- Flint, L.E., Matrix properties of hydrogeologic units at Yucca Mountain, Nevada, U.S. Geological Survey OFR 96-xxx, U.S. Geological Survey, 1996 (in preparation).
- Flint, A.L., H.A. Hevesi, and L.E. Flint, Conceptual and numerical model of infiltration for the Yucca Mountain area, Nevada, U.S. Geological Survey WRI 96-xxxx, U.S. Geological Survey, 1996 (in preparation).
- Flint, L.E., A.L. Flint, C.A. Rautman, and J.D. Istok, Physical and hydrologic properties of rock outcrop samples at Yucca Mountain, Nevada, U.S. Geological Survey Report OFR-95-280, U.S. Geological Survey, 1996b.
DTN: GS940808312231.008

Geological Model Development and Vertical Layering Scheme for the Numerical Grid

- Hevesi, J.A., D.S. Ambos, and A.L. Flint, A preliminary characterization of the spatial variability of precipitation at Yucca Mountain, Nevada, Proceedings of the Fifth Annual International Conference High Level Radioactive Waste Management, Sponsored by the American Nuclear Society and American Society of Civil Engineers, Las Vegas, Nevada, May 22-26, pp. 2520-2529, 1994.
- Montazer, P. and W.E. Wilson, Conceptual hydrologic model of flow in the unsaturated zone, Yucca Mountain, Nevada, Water Resources Investigations Report 84-4355, U.S. Geological Survey, p.55, 1984.
- Moyer, T.C., and J.K. Geslin, Lithostratigraphy of the Calico Hills Formation and Prow Pass Tuff (Crater Flat Group) at Yucca Mountain, Nevada. U.S. Geological Survey Report OFR 94-460, , U.S. Geological Survey, 1995a.
DTN: GS940608314211.028
- Moyer, T.C., J.K. Geslin, and L.E. Flint, Stratigraphic relations and hydrologic properties of the Paintbrush Tuff nonwelded (Ptn) hydrologic unit, Yucca Mountain Nevada, U.S. Geological Survey Report OFR 95-397, U.S. Geological Survey, 1995b.
- Muller, DC, and J.E. Kibleer, Preliminary analysis of geophysical logs from the WT series of drill holes, Yucca Mountain, Nye County, Nevada, U.S. Geological Survey Report OFR 86-46, U.S. Geological Survey, 1985.
- Nelson, P.H., D.C. Muller, U. Schimschal, and J.E. Kibler, Geophysical logs and core measurements from forty boreholes at Yucca Mountain, Nevada, 1989.USGS MAP GP-1001.
DTN: GS920108314213.001
- Nelson, P.H., Saturation levels and trends in the unsaturated zone, Yucca Mountain, Nevada, Proceedings: Fifth International High Level Radioactive Waste Management Conference, May 23-26, Las Vegas, Nevada, pp. 2774-2781, 1994.
- Nimick, F.B. and Williams, R.L., A three-dimensional geologic model of Yucca Mountain, Southern Nevada, SAND83-2593, 1984.
- Nelson, P.H., Computation of porosity and water content from geophysical logs, Yucca Mountain, Nevada, U.S. Geological Survey Report OFR96-078, U.S. Geological Survey, 1996.
- Ortiz, T.S., R.L. Williams, F.B. Nimick, B.C. Whittet, and D.L. South, A three-dimensional model of reference thermal/mechanical and hydrologic stratigraphy at Yucca Mountain, Southern Nevada, SAND84-1076 (SNSAND84107600.000), 1985.
- Robinson, B.A., A.V. Wolfsberg, G.A. Zyvoloski, and C.W. Gable, An unsaturated zone flow and transport model of Yucca Mountain, LA-Milestone 3468 (Draft), 1995.

Geological Model Development and Vertical Layering Scheme for the Numerical Grid

Scott, R.B., and J. Bonk, Preliminary geologic map of Yucca Mountain, Nye County, Nevada, with geologic sections, U.S. Geological Survey Report OFR-84-494, U.S. Geological Survey, 1984.

Tucci, P, and D.J. Burkhardt, Potentiometric-surface map (1993), Yucca Mountain and Vicinity, Nevada, U.S. Geological Survey WRI95-4149, U.S. Geological Survey, 1995.

Wittwer, C.S., G.S. Bodvarsson, M.P. Chornack, A.L. Flint, L.E. Flint, B.B. Lewis, R.W. Spengler, and C.A. Rautman, Design of a three-dimensional site-scale model for the unsaturated zone at Yucca Mountain, Nevada, Proceedings of the Third Annual International Conference on High Level Radioactive Waste Management, (American Nuclear Society and American Society of Civil Engineers, Eds.), Las Vegas, Nevada, V. 1, pp. 263-271, 1992.

Wittwer, C., G. Chen, G.S. Bodvarsson, M. Chornack, A. Flint, L. Flint, E. Kwicklis, and R. Spengler, Preliminary development of the LBL/USGS three-dimensional site-scale model of Yucca Mountain, Nevada, Lawrence Berkeley National Laboratory Report LBL-37356, UC-814, Lawrence Berkeley National Laboratory, Berkeley, CA, 1995.

Zelinski, WP, and Clayton, RW. (CRWMS M&O), A 3D geological framework and integrated site model of Yucca Mountain: Version ISM1.0., Doc. ID B00000000-01717-5700-00002 Rev 1, July 11, 1996.

References for Borehole Lithostratigraphic Contacts

N/A = This information not available 08/96.

Report Name/Data Source	QA Status ¹	DTN/ACC.#
Bentley, C.B., J.H. Robison, and R.W. Spengler, 1983, Geohydrologic data for test well USW H-5, Yucca Mountain area, Nye County, Nevada: USGS Open-File Report 83-853, 34 p.	NQA	GS910908312132.002 NNA.19890804.000
Byers, F. M., Jr., and R. G. Warren, 1983, Revised Volcanic stratigraphy of drill hole J-13, Fortymile wash, Nevada, based on petrographic modes and chemistry of phenocrysts: LosAlamos National Laboratory Report LA-9652-MS, 23 p.	NQA	LA000000000045.001 NNA.19870406.0422
Byers, F. M., R. W. Orsak, and M. P. Chornack, 1994, Preliminary report on geology of drillhole USW-GA1, Yucca Mountain, Nevada Test Site (unpublished report): in Preliminary Source Information, Stratigraphy, and Lithologic Logs for Several Yucca Mountain Boreholes: Letter from L. R. Hayes (USGS) to S. B. Jones (DOE), June 6, 1994.	NQA	N/A N/A

Geological Model Development and Vertical Layering Scheme for the Numerical Grid

Carr, M. D., S. J. Waddell, G. S. Vick, J. M. Stock, S. A. Monsen, A. G. Harris, B. W. Cork, and F. M. Byers, Jr., 1986, Geology of drill hole UE25p#1: A test hole to pre-Tertiary rocks near Yucca Mountain, southern Nevada: U.S. Geological Survey Open-file Report 86-175, 87 p.	NQA	GS930283117461.002 HQS.19880517.2633
Craig, R. W., R. L. Reed, and R. W. Spengler, 1983, Geohydrologic data for well USW H-6, Yucca Mountain area, Nye County, Nevada: U.S. Geological Survey Open-File Report 83-856, 39 p.	NQA	GS910908312132.001
Geldon, A. A., 1991, Preliminary hydrogeologic assessment of boreholes UE-25 c#1, UE-25c#2, and UE-25 c#3, Yucca Mountain, Nye County, Nevada: unpublished U.S. Geological Survey Water Resources Investigations Report 92-4016, 176 p.	NQA	GS930308312313.002 NNA.930120.0040.
Geslin, J.K. and Moyer, T. C., 1994, Summary of lithologic logging of new and existing boreholes at Yucca Mountain, Nevada, March 1994 to June 1994: U.S. Geological Survey Open-File Report 94-451, 16 p. [for NRG-2c, NRG-2d, NRG-7/7a in order:]	QA	GS940308314211.012
	QA	NNA.19940504.0010
	QA	GS940308314211.013 NNA.19940504.0013 GS940408314211.020 NNA.19940629.0032
Geslin, J., T. Moyer, and D. C. Buesch, 1994, Summary of Lithologic Logging of New and Existing Boreholes at Yucca Mountain, Nevada, August 1993 to February 1994: U.S. Geological Survey Open-File Report 94-342, 68 p.	QA	GS940308314211.009 MOL.19940810.0011
Kume, J., and D.P. Hammermeister, 1991, Geohydrologic data from drill-bit cuttings and rotary cores from test hole USW UZ-13, Yucca Mountain area, Nye County, Nevada: U.S. Geological Survey Open-File Report 90-362, 30 p.	NQA	GS920808312232.001 NNA.19901015.0196
Kume, J., and D.P. Hammermeister, 1990, Geohydrologic data from test hole USW UZ-7, Yucca Mountain area, Nye County, Nevada: U.S. Geological Survey Open-File Report 88-465, 37 p.	NQA	GS900908312232.001 MOL.19950119.0049
Lobmeyer, D.H., M.S. Whitfield, Jr., R.R. Lahoud, and L. Bruckheimer, 1983, Geohydrologic Data for Test Well UE-25b#1H, Nevada Test Site, Nevada: U.S. Geological Survey Open-File Report 83-855, 52 p.	NQA	GS930408312313.004 NNA.19890511.0124
Loskot, C.L., and D.P. Hammermeister, 1992, Geohydrologic data from test holes UE-25 UZ#4 and UE-25 UZ#5, Yucca Mountain area, Nye County, Nevada: U.S. Geological Survey Open-File Report 90-369, 56 p.	NQA	GS921008312211.008 NNA.19911219.0001
Lugo, C. L., 1995, Distribution of Field Borehole Summary for UE-25 ONC#1, Letter: Lugo, C. L. (SAIC) to Gridley, W.A.. (DOE), January 6, 1995.	NQA	N/A N/A
Maldonado, F., and S.L. Koether, 1983, Stratigraphy, structure, and some petrographic features of Tertiary volcanic rocks at the USW G-2 drill hole, Yucca Mountain, Nye County, Nevada: U.S. Geological Survey Open-File Report 83-732, 83 p.	NQA	GS930208314211.008 NNA.19870506.0143
Moyer, T. C., and G. Mongano, 1994a, Graphical lithologic log of borehole USW SD-9 from the surface to the base of the Paintbrush Group.	QA	GS940808314211.041 MOL.19950522.0208

Geological Model Development and Vertical Layering Scheme for the Numerical Grid

Moyer, T. C., and G. Mongano, 1994b, Graphical lithologic log of borehole USW SD-9 from the base of the Paintbrush Group to total depth.	QA	GS941108314211.052 MOL.19950505.0057
Moyer, T. C., J.K. Geslin, and D. C. Buesch, 1995, Summary of Lithologic Logging of New and Existing Boreholes at Yucca Mountain, Nevada, July 1994 to November 1994: USGS OFR 95-102, 27 p.	QA	GS941208314211.060 MOL.19960222.0335
Moyer, T.C., and J.K. Geslin, 1994a, Table of basal lithologic contacts in borehole USW UZN-11.	QA	GS940308314211.010
Moyer, T.C., and J.K. Geslin, 1994b, Table of lithologic contacts in boreholes USW UZN-15, USW UZ-N16 and USW UZ-N17.	QA	GS940308314211.019 MOL.19941101.0061
Moyer, T.C., and J.K. Geslin, 1994c, Table of lithologic contacts in borehole USW UZ-N36.	QA	GS940308314211.018 MOL.19941101.0062
Moyer, T.C., and J.K. Geslin, 1994d, Table of lithologic contacts in borehole USW UZ-N38.	QA	GS940308314211.011 MOL.19941101.0063
Moyer, T.C., and J.K. Geslin, 1994e, Table of lithologic contacts in borehole USW UZN#63.	QA	GS940308314211.017 MOL.19941101.0064
Moyer, T.C., and J.K. Geslin, 1994f, Table of lithologic contacts in borehole USW UZ-N64.	QA	GS940308314211.016 MOL.19941101.0065
Moyer, T. C., J. K. Geslin, and D. Buesch, 1993, Summary lithologic descriptions of the upper Tiva Canyon formation and tuff unit "x" in the North Ramp area, 26 p.	QA	GS931108314211.044 NNA.19940217.0147
Norris, A.E., F.M. Byers, Jr., and T.J. Merson, 1986, Fran Ridge horizontal coring summary report, hole UE-25h#1, Yucca Mountain area, Nye County, Nevada: Los Alamos National Laboratory Report LA-10859-MS, 78 p.	NQA	LA000000000047.001 NNA.19891129.0072
Rautman, RA, and Engstrom, DA. 1996. Geology of the USW SD-7 Drill Hole, Yucca Mountain, Nevada. Sandia National Laboratory Letter Report SLTR-96-000X. SNL Report SAND96-1474.	TQA	NA NA
Rautman, RA, and Engstrom, DA. 1996. Geology of the USW SD-12 Drill Hole, Yucca Mountain, Nevada. Sandia National Laboratory Letter Report SLTR-96-000X. SNL Report SAND96-1368	TQA	NA NA
Rush, F. E., W. Thordarson, and L. Bruckheimer, 1983, Geohydrologic and drill-Hole data for test well USW H-1, adjacent to Nevada Test Site, Nye County, Nevada: U.S. Geological Survey Open-File Report 83-141, 38 p.	NQA	GS900908312211.001 NNA.19870519.0103
Rush, F. E., W. Thordarson, and D. G. Pyles, 1984, Geohydrology of test well USW H-1, Yucca Mountain, Nye County, Nevada: U.S. Geological Survey Water-Resources Investigations Report 83-4032, 56 p.	NQA	GS920408312314.011 NNA.19870518.0067

Geological Model Development and Vertical Layering Scheme for the Numerical Grid

Scott, R. B., and M. Castellanos, 1984, Stratigraphic and structural relations of volcanic rocks in drill holes USW GU-3 and USW G-3, Yucca Mountain, Nye County, Nevada: U.S. Geological Survey Open-File Report 84-491, 121 p.	NQA	GS920908314211.002 NNA.19890804.0017
Spengler, R.W., 1994a, Lithologic log of drill hole UE-25WT#4.	NQA	N/A NNA.19940608.0296
Spengler, R.W., 1994b, Lithologic log of drill hole USW WT-11.	NQA	N/A NNA.19940526.0144
Spengler, R.W., 1994c, Lithologic log of drill hole UE-25WT#12.	NQA	N/A NNA.19940608.0298
Spengler, R.W., 1994d, Lithologic log of drill hole UE-25WT#13.	NQA	N/A NNA.19940608.0292
Spengler, R.W., 1994e, Lithologic log of drill hole UE-25WT#14.	NQA	N/A NNA.19940608.0301
Spengler, R.W., 1994f, Lithologic log of drill hole UE-25WT#15.	NQA	N/A NNA.19940608.0293
Spengler, R.W., 1993a, Preliminary lithologic well reports; USW WT-1, 2, 7, 10 and UE-25 WT-3, 16, 17, 18.	NQA	GS930208314211.004 NNA.930315.0336
Spengler, R.W., 1993b, , Preliminary lithology well report for UE25 WT-6.	NQA	GS930208314211.006 NNA.930315.0336
Spengler, R.W., 1993c, Preliminary lithologic log of test hole UE-25 UZ#5.	NQA	GS930108314211.002 NNA.930315.0334
Spengler, R.W., 1993d, , Preliminary Lithologic Log of Test Hole USW UZ#6.	NQA	GS930208314211.006 NNA.940512.0001
Spengler, R.W., 1993e, Preliminary lithologic log of test holes [sic] USW UZ#1, Nevada.		N/A NNA.940405.0355
Spengler, R.W., 1992, Lithologic log of test hole USW UZ-13, Nevada.	NQA	N/A NNA.19920629.0053
Spengler, R.W., 1985, Condensed log of UE25 UZ-4.	NQA	N/A NNA.940328.0225
Spengler, R. W., 1983, H-4 lithologic log.	NQA	N/A NNA.900820.0131

Geological Model Development and Vertical Layering Scheme for the Numerical Grid

Spengler, R. W., and M. P. Chornack, 1984, Stratigraphic and structural characteristics of volcanic rocks in core hole USW G-4, Yucca Mountain, Nye County, Nevada, with a section on Geophysical logs by D.C. Muller and J. E. Kibler: U.S. Geological Survey Open-File Report 84-789, 77 p.	NQA	GS920908314211.003 NNA.19890804.0012
Spengler, R. W., and J. G. Rosenbaum, 1980, Preliminary interpretations of geologic results obtained from boreholes UE25a-4, -5, -6, and -7, Yucca Mountain, Nevada Test Site: U.S. Geological Survey Open-File Report 80-929, 33 p.	NQA	GS900908314213.002 NNA.19890823.0106
Spengler, R. W., F. M. Byers, Jr., and J. B. Warner, 1981, Stratigraphy and structure of volcanic rocks in drill hole USW-G1, Yucca Mountain, Nye County, Nevada: U.S. Geological Survey Open-File Report 81-1349, 50 p.	NQA	GS930208314211.005 NNA.19870406.0222
Spengler, R. W., D. C. Muller, and R. B. Livermore, 1979, Preliminary report on the geology and geophysics of drill hole UE25a-1, Yucca Mountain, Nevada Test Site: U.S. Geological Survey Open-File Report 79-1244, 43 p.	NQA	GS920908314211.004 NNA.19870406.0349
Stellavato, N. 1995, written communication, Draft UE-25 ONC#1 Geology by Moyer, T. and McMaster, L., Letter: Stellavato to Tynan, M. dated 3/17/95, Nuclear Waste Repository Project Office, Box 2389, Pahrump, Nevada, 3p.	NQA	N/A N/A
Thordarson, W., F. E. Rush, R. W. Spengler, and S. J. Waddell, 1984, Geology and drill-hole data for test well USW H-3, Yucca Mountain, Nye County, Nevada: U.S. Geological Survey Open-File Report 84-149, 28 p.	NQA	GS900908312312.001 NNA.19870406.0056
Whitfield, M. S., Jr., C. M. Cope, and C. L. Loskot, 1993, Borehole and geohydrologic data for test hole USW UZ-6, Yucca Mountain area, Nye County, Nevada: U.S. Geological Survey Open-File Report 92-28, 36 p.	NQA	GS910808312232.002NN A.19920123.0088
Whitfield, M. S., Jr., W. Thordarson, and D. P. Hammermeister, 1990, Drilling and geohydrologic data for test hole USW UZ-1, Yucca Mountain, Nye County, Nevada: U.S. Geological Survey Open-File Report 90-354, 40 p.	NQA	GS930608312232.016 NNA.19900622.0450
Whitfield, M. S., Jr., E. P. Eshom, W. Thordarson, and D. H. Shaefer, 1985, Geohydrology of rocks penetrated by test well USW H-4, Yucca Mountain, Nye County, Nevada: U.S. Geological Survey Water-Resources Investigations Report 85-4030, 33 p.	NQA	GS920408312314.008 NNA.19870407.0328
Whitfield, M. S., Jr., W. Thordarson, and E. P. Eshom, 1984, Geohydrologic and drill-hole data for test well USW H-4, Yucca Mountain, Nye County, Nevada: U.S. Geological Survey Open-File Report 84-449, 39 p.	NQA	GS900908312312.002 NNA.19870407.0317
Zimmerman, C.L., and D.C. Buesch, 1995, Graphical lithologic log of borehole USW UZ-7a, 4 p.	QA	GS950908314211.034 N/A
¹ QA=Qualified Data; NQA= Not QualifiedData; TQA=Qualified Data Package to be submitted to TDB by 9/96.		

SATURATION AND CAPILLARY PRESSURE ANALYSIS

T.M. Bandurraga, S. Finsterle, and G.S. Bodvarsson

August 1996

3.1 Introduction

The role of the three-dimensional site-scale model of the unsaturated zone at Yucca Mountain (UZ model) is to provide a baseline description of the ambient hydrologic state. Once that has been achieved, the model can then be used to calculate percolation fluxes within the mountain. It can also be used to predict the response of heat, gas, and moisture flows to perturbations such as long-term climate changes and in performance assessment activities.

3.1.1 UZ Model Calibration

A critical step in the development of the UZ model is the calibration against measurements of gas, moisture, and heat from the mountain. The calibration enables the model to simulate ambient conditions and develops confidence in the predictive capabilities of the model. The available measurements which characterize ambient conditions in the UZ at Yucca Mountain consist of saturation, capillary pressure, temperature, pneumatic data, ESF data, and ages and distributions of environmental isotopes.

These data can all be used to calibrate the UZ model and determine hydrogeologic parameters. The environmental isotopes data are obtained from samples obtained from boreholes and in the ESF. The ESF samples indicate the presence of structural features which act as fast pathways for pulsed infiltration. The temperature data have been gathered through borehole logging after drilling or with sensors installed as part of borehole instrumentation programs. The temperature data are related to the thermal conductivities of the geologic layers and can be affected by infiltration rates.

The pneumatic data have been gathered from the borehole instrumentation programs, and provide diffusivities for the various geologic formations. The diffusivities can be converted to permeability estimates. The permeability results are generally considered to be primarily due to the contribution of gas flowing through fractures.

The matrix saturation and capillary pressure data are usually obtained from borehole core samples, although in the past some measurements have been made on borehole cuttings. Other saturation estimates can be made from geophysical logging of the boreholes. Additional capillary pressure measurements have been obtained from sensors installed as part of the borehole instrumentation program. The data are indicative of conditions in the matrix in response to historic infiltration rates.

3.1.2 Saturation and Capillary Pressure Use and Limitations

Although matrix saturation and capillary pressure data characterize the conditions in response to historic infiltration rates, the uncertainty associated with those rates is high. Previous estimates of net infiltration at Yucca Mountain have ranged from 0.01 to more than 20 mm/yr with various approaches. It is uncertain how much the temporal variability of the precipitation affects the percolation flux at depth within the mountain or how much the historic infiltration pattern has changed. Therefore, it is difficult to pick one rate which can be used in the calibration to determine the effective hydrogeologic parameters.

There are also uncertainties associated with the data. The drilling process creates extreme physical conditions at the drill-bit which may affect saturations and capillary pressures. The sample handling process can dry out the samples and bias the measurements. Finally, there are measurement resolution limits and uncertainties in the laboratory. Uncertainties are also applicable to the in-situ measurements of capillary pressures. The sensors are installed in ungrouted borehole intervals which can be more than ten meters, so that they measure average conditions across the layer rather than point measurements. The saturation estimates based on geophysical data combine the errors involved in measuring both the total and water-filled porosity with logging, so that the uncertainties can be quite large. The data also have to be corrected in formations that have a large percentage of lithophysal cavities which do not provide connected pathways for moisture or gas flow.

3.1.3 Objectives of Saturation and Capillary Pressure Calibration

The objectives of this study can be summarized as follows:

1. Examine the ability of the UZ model of Yucca Mountain to reproduce saturation and capillary pressure measurements.
2. Calibrate the UZ model or various submodels against saturation and capillary pressure data using inverse modeling techniques.
3. Evaluate the uncertainties of the developed set of model-related hydrogeologic parameters and discuss their impact on subsequent modeling efforts.
4. Estimate the most likely infiltration flux through the matrix based on the saturation and capillary pressure data.
5. Develop a Q set of parameters which can be used in site assessment modeling activities by project scientists.

3.1.4 Previous Work

A previous calibration effort for the UZ model was presented in Ahlers et al. (1995). This calibration effort used the ECM formulation of the model presented in Wittwer et al. (1995) and relied heavily on limited non-Q data. The results of the calibration were also affected by the smaller number of model layers representing geological variability in the unsaturated zone. Numerous Q

Saturation and Capillary Pressure Analysis

saturation and capillary pressure data are presently available from project scientists, and the UZ model grid has been revised as discussed in Chapter 2 (Bandurraga et al., 1996) of this report to explicitly include the important geological layers affecting flow patterns in the UZ.

3.1.5 Model Calibration Issues

Calibrating a numerical model against field data requires assessing potential errors and uncertainties of both the data and the model. Table 3.1.5-1 presents a summary of the uncertainties which can affect the calibration process.

Table 3.1.5-1 Data and Numerical Uncertainties	
Data Uncertainties	Numerical Grid and Modeling Uncertainties
<u>Type</u>	<u>Type</u>
Accuracy, precision, and reproducibility Biased estimates Systematic errors	Numerical Dispersion and Diffusion
<u>Source</u>	<u>Source</u>
Sample collection and preparation Measurement procedures Data processing, interpretation Systematic errors and outliers	Grid Refinement Flow Dimensionality Initial and Boundary Conditions Numerical Solution Scheme

Besides data and model uncertainties, a number of difficulties arise when actually comparing field data to model results. Conceptual and numerical differences exist between the values obtained in the field and the corresponding model variables. The most obvious differences are due to the scaling problem. The saturation data, for example, reflect conditions on a local scale on the order of meters, whereas the model-calculated-values represent average saturations on the scale of an individual model grid block which can be on the order of tens of meters. In a fractured system, there is also a conceptual difference between the (indirectly) measured saturation and the model calculations using an equivalent continuum approximation.

Another key problem is heterogeneity, and the limited degree to which it can be resolved in a three-dimensional site-scale model. For example, boreholes UZ#4 and UZ#5, which are only about 40 m apart, have considerably different saturation and capillary pressure profiles. However, both are represented by the same vertical column of grid blocks in the UZ model. Although this may suggest that there is insufficient horizontal discretization in the numerical model, the problem is really the scale of the heterogeneities which can be resolved by a site-scale model. The UZ model represents vertical heterogeneities in geologic formations on the scale of tens of meters such as broad alteration fronts, faults, and average fracturing intensity. It is not expected to resolve heterogeneities on the order of meters such as localized increases in fracturing or areas of alteration.

3.1.6 Chapter Organization

The chapter is organized so that there is a review of the saturation and capillary pressure data collected by the project in Section 3.2. Section 3.3 discusses the modeling approach, especially the development of an appropriate submodel to simulate moisture flow under steady-state conditions. The submodel preparation and calibration results for a range of uniform infiltration rates are presented in Section 3.4. Section 3.5 presents the approaches used in performing sensitivity analyses of the uniform rate calibration and the results of those analyses. Concluding remarks are provided in Section 3.6.

3.2 Data Description

3.2.1 Available Borehole and Fracture Data

This section briefly reviews the borehole and fracture data set available from project scientists. This data set was used to estimate the model-related hydrogeologic parameters through inverse modeling. There are two types of borehole data used in this study, matrix saturation data, and matrix capillary pressure measurements. A summary of the matrix data available from borehole core samples for use in the calibration is given in Table 3.2.1-1. Saturation measurements are available for all of the boreholes, while capillary pressure data are available for boreholes SD-7, SD-9, and UZ-14. The reference is the project data tracking number from the Technical Data Base.

Table 3.2.1-1 Saturation and Water Potential Borehole Data from USGS. (L. Flint, Principal Investigator)				
Borehole	Saturation	Water Potential	Q Status	Reference
SD-7	*	*	Y	YMP DTN GS951108312231.009
SD-9	*	*	Y	YMP DTN GS950308312231.004
SD-12	*		Y	YMP DTN GS950308312231.002
UZ-14	*	*	Y	YMP DTN GS950308312231.005
UZ#16	*		Y	YMP DTN GS940508312231.006

The saturation and capillary pressure data summarized in Table 3.2.1-1 were obtained from core samples. Saturation was derived by first measuring a composite gravimetric water content using oven-drying methods. Bulk- and grain-density measurements were performed to calculate porosity and saturation. Saturation data are also available for boreholes NRG-6 and NRG-7a, but the principal investigator for the laboratory measurements reported that sample disturbance led to significant drying-out of the cores prior to saturation measurements (L. Flint, USGS, personal communication, June, 1996). Therefore, the data from these boreholes were not used in the calibration.

The saturation data are available using two different drying ovens - a relative humidity oven at a temperature of about 65 degrees C and a 105 degrees C oven. The hotter oven drives off the structural and bound water in the pores, and typically provides higher saturation estimates than the results from the relative humidity oven. However, this structural and bound water is not thought to contribute to flow through the matrix pores. Therefore, the relative humidity oven saturation results were used in the calibration efforts. The 105 degrees C oven results were used for borehole SD-7, however, because some zeolitic core sample relative humidity results were unreliable.

Capillary pressure is defined as the negative of matric potential, and was measured on the core samples using thermocouple psychrometers. The thermocouple psychrometer measures the water potential (sum of matric and osmotic potentials). However, in non-saline porous media the osmotic component can often be neglected. For the purposes of this chapter, capillary pressures are positive, with drier conditions shown by larger pressures for a given matrix sample. A plot of the capillary pressure data (see, for example, Figure 3.4.3-1) shows that the instrument resolution near saturation is about 1.26 bars. As the samples become drier (matric potentials decrease), the uncertainties of the measurements increase significantly and vary widely within an assumed homogeneous geologic layer. However, trends in the data are apparent, with lower capillary pressures measured in non-welded vitric layers, and higher values found in densely welded or altered layers.

The capillary pressures are problematic in that relatively high values were measured in cores from known zones of perched water in boreholes. It is expected that perched water zone samples should be fully saturated with relatively low pressures. J. Rousseau of the USGS has instrumented a number of boreholes at Yucca Mountain and is collecting data on water potentials from them. LBNL received a preliminary data set containing the data from these boreholes in July, 1996. These data will be Q by the end of FY96.

The psychrometers providing the in-situ water potential measurements are placed in ungrouted intervals with widths on the order of ten meters, and so they provide average measurements of conditions in the vicinity of the sensor. When compared to arithmetically-averaged layer values from the core sample results, the in-situ measurements are much smaller (see, for example, Figure 3.5.4-1). Rousseau et al. (1996) have shown an extensive analysis of water potential data. The study indicates that any sample mishandling of the low porosity cores can lead to dry-out and have a significant effect on water potentials. This may account for some of the data variability reported for an assumed relatively homogeneous geologic layer.

Limited non-Q saturation and water potential measurements are also available from previous studies of Yucca Mountain. These data were used in the pre-

vious calibration effort reported in Ahlers et al. (1995). However, they were not used in this study.

Non-Q saturation data have been developed from calculations based on porosity and water content analyses from geophysical logging for 25 boreholes at Yucca Mountain. There is also the possibility that these data might become Q in the future. Q saturation data from geophysical logging from a number of boreholes are presently being developed by the staff of the YMP M&O, but were not available at the time of this study. These Q geophysical data overlap with some of the boreholes with core sample measurements, so there is some basis for comparison of the data already used in this calibration and the geophysical data presently becoming available. The Q data also overlap with some of the presently non-Q data from the 25 boreholes.

A careful analysis of the geophysical data must be performed prior to their use to compare the saturation estimates with Q core sample data and resolve any differences. One problem is that the log data need to be corrected for the presence of lithophysal cavities found in some layers of the TSw which bias the porosity estimates. Preliminary comparisons of saturation estimates based on log data to core sample saturations for borehole SD-9 show significant differences.

The fractures at Yucca Mountain are not easily characterized through direct measurements because they vary so widely in length, orientation, connectivity, aperture width, amounts and types of coatings, and other important parameters. The few available saturation and capillary pressure measurements (Persoff and Pruess, 1995; Thamir et al., 1993) from specific fractures are not expected to be representative of conditions in the complex fracture networks at Yucca Mountain. Therefore, no fracture saturation or capillary pressure data were used in the calibration.

The calibration effort described in this chapter relied upon the Q matrix saturation and water potential data outlined in Table 3.2.1-1 to establish ambient hydrogeological conditions. However, the matrix property data sets for the bottom portions of boreholes SD-7 and -12 will not be Q until they are submitted in September, 1996. The preliminary in-situ water potential data provided by J. Rousseau of the USGS will also be Q data in September, 1996. The non-Q matrix data described above were not used to corroborate the calibration effort at this time. It is hoped that Q geophysical saturation estimates will be available for future calibration efforts

3.2.2 Matrix and Fracture Hydrogeologic Parameters

The saturation and capillary pressure data depict the ambient hydrologic state of the unsaturated zone at Yucca Mountain. The primary use of these data in a calibration effort is to develop a set of hydrogeologic parameters which will allow the model to simulate ambient conditions. However, since the saturation and capillary pressure data are only available for a few of the boreholes, the

solution to the inverse problem is non-unique and potentially unstable. One way to reduce non-uniqueness is to introduce prior information (Carrera and Neuman, 1986), i.e., measurements of the parameters themselves are used as additional data points. Differences between the measured and estimated parameters values constitute a plausibility criterion for the inversion. Furthermore, if no sensitive data are available, this approach retrieves the measured parameter value as the best estimate, making the inversion more stable and reducing estimation uncertainty.

Extensive measurements of the hydrogeologic parameters have been performed with core samples and in-situ analyses. In addition, data analyses and model simulations have provided additional estimates of hydrogeologic parameters. These parameters include matrix and fracture permeabilities estimated with hydraulic conductivity and air permeability testing, and matrix van Genuchten fitting coefficients and residual saturations obtained from desorption curve measurements as discussed in the references provided in the following discussion.

Many of the original hydrogeological parameters used in modeling studies of Yucca Mountain were published by SNL staff in reports by Klavetter and Peters (1986, 1987) and Peters et al. (1986). These and other data were later used in an evaluation of matrix and fracture properties and the results provided by Schenker et al. (1995) in support of the TSPA-93 (Wilson et al., 1994). The TSPA-95 document (M&O, 1995) refers to these previous documents in the discussion on hydrogeologic parameters. The parameters have been used in a number of modeling studies and code comparisons (see, for example, Ho et al., 1995).

The USGS testing program has also generated a large data set of hydrogeologic parameters. Saturated zone test programs have provided estimates of fracture conductivities. Outcrop transect studies have provided matrix properties such as porosity, bulk density, conductivities and van Genuchten fitting parameters (Flint and Flint, 1990; Flint and Flint, 1993). Other reports provided the results of borehole sample measurements (for example, Kume et al., 1990, 1991; Loskot et al, 1992; Loskot, 1993).

However, many of the data sets discussed above are non-Q. At this time in the project, work which is to be used in site suitability studies must be developed primarily under the QA program. This is not to say that the non-Q data are inaccurate or cannot be used to confirm the work done with Q data. In many cases, data which are non-Q could potentially become Q data if documentation exists that the work was done according to present Q requirements. However, there has been only a limited effort to try to qualify non-Q data.

The calibration effort described in this chapter relied upon the Q matrix hydrogeologic properties developed by L. Flint (1996, in prep.) of the USGS. This data set provides properties for all of the layers used in the site-scale model

as described in the following section. These data will be Q by the end of September, 1996. The non-Q property sets summarized above were not used to confirm the analyses in any way. Unfortunately, the fracture data sets are not as robust, as described in Section 3.2.2.2. Q fracture permeabilities are available from a number of in-situ measurements and modeling studies. However, the fracture van Genuchten parameters used in this study were obtained from the non-Q TSPA-93 data set.

3.2.2.1 Matrix Properties

With the emphasis on Q data, the USGS has recently done extensive matrix property measurements on borehole core samples. The Q data sets include porosity, bulk density, saturated hydraulic conductivity, van Genuchten fitting coefficients (obtained from desorption curves), and residual saturation for core samples from a number of boreholes. The numerous measurements have characterized the geologic formations important to unsaturated zone flow with more detail than was previously possible. Based on these data, representative values for the different layers have been determined by the USGS (Flint, 1996, in prep.). These values are considered to be the best available data set and are therefore used as the initial estimates for the calibration. Table 3.2.2-1 presents the correlation of the units used in TSPA93 and the geologic formations included in the units. Table 3.2.2-2 presents a comparison of the parameters from the TSPA-93 data set (non-entropy fit values) and the Flint (1996, in prep.) data which was used as the input to the calibration.

Table 3.2.2-1 TSPA Unit Designation and Correlation with Geologic Formations		
TSPA93 Unit Number	Layer Description	Buesch et al. (1995) Designation
1	Tiva Canyon Welded	Tcpxxx
2	Paintbrush non-welded	Tcpv1, Tpbt4, Tpy, Tpbt3, Tpp, Tpbt2, Tptrv3
3c	Topopah Spring welded- composite	Tpboxx
3r	Topopah Spring welded- repository	Tptpmn, Tptpln, Tptpln
4	Topopah Spring vitrophyre	Tptpv3
5	Calico Hills/Prow Pass nonwelded-vitric	Ta, Tcp (nwv)
6	Calico Hills/Prow Pass nonwelded-zeolitic	Ta, Tcp (nwz)
7	Prow pass welded	Tcp-(w)
8	Bullfrog welded	Tcb-(w)
9	Bullfrog nonwelded	Tcb-(nw)
10	Tram welded	Tct-(w)
nwz= non-welded zeolitic nwv= non-welded vitric		

Saturation and Capillary Pressure Analysis

Table 3.2.2-2 Matrix Hydrogeologic Parameter Comparison (Flint 96=Flint, 1996, in prep.)							
Geologic Layer(s)	TSPA-93 Unit	Permeability (m ²)		van Genuchten alpha (1/bars)		van Genuchten m	
Buesch et al. (1995)		TSPA-93	Flint 96	TSPA-93	Flint 96	TSPA-93	Flint 96
Upper Tpcxxx	1	3.7E-17	1.5E-19	0.22	0.34	0.383	0.20
Middle Tpcpxx	1	3.7E-17	5.4E-18	0.22	0.12	0.383	0.23
Tpcpv3,2	1	3.7E-17	2.2E-17	0.22	0.023	0.383	0.44
Tpcpv1, Tpb4	2	5.5E-14	4.0E-13	2.49	3.65	0.617	0.22
Tpy	2	5.5E-14	3.0E-16	2.49	0.76	0.617	0.49
Tpb3	2	5.5E-14	5.2E-14	2.49	2.59	0.617	0.24
Tpp	2	5.5E-14	8.8E-14	2.49	3.41	0.617	0.30
Tpb2, Tptrv3	2	5.5E-14	4.2E-13	2.49	9.80	0.617	0.23
Tptrv2,1	3c	2.4E-17	1.6E-16	0.30	0.34	0.442	0.20
Tptrn	3c	2.4E-17	1.7E-16	0.30	2.04	0.442	0.25
Tptrl, Tptpul	3c	2.4E-17	2.0E-17	0.30	0.66	0.442	0.25
Tptpmn	3r	2.4E-17	4.0E-18	0.30	0.064	0.442	0.32
Tptpll	3r	2.4E-17	2.3E-17	0.30	0.27	0.442	0.23
Tptpln	3r	2.4E-17	9.6E-17	0.30	0.047	0.442	0.42
Tptpv3	4	2.4E-18	5.0E-18	0.03	0.010	0.589	0.37
Tptpv2,1; Tpb1(z)	6	1.9E-17	5.4E-16	0.19	0.019	0.429	0.36
Ta(z)	6	1.9E-17	4.5E-18	0.19	0.39	0.429	0.22
Thbt, Prow Un. 4 (z)	6	1.9E-17	8.4E-18	0.19	0.015	0.429	0.48
Prow Un. 3	7	2.6E-16	3.8E-17	0.18	1.82	0.857	0.31
Prow Un. 2,1; Tpb1(z)	6	2.6E-16	1.7E-17	0.18	0.18	0.857	0.31
Tptpv2,1; Tpb1	5	1.8E-15	1.6E-12	0.53	9.80	0.636	0.23
Ta	5	1.8E-15	5.5E-14	0.53	9.80	0.636	0.23

The permeability values presented in Table 3.2.2-2 are relatively similar, considering that the TSPA-93 values are not provided for as many of the individual geologic formations as the recent Q USGS measurements. The van Genuchten alpha parameters can be quite different, however, especially for the TCw basal vitrophyre, some of the more densely welded formations in the TSw, and zeolitic layers in Tpb1 and Tptpv1. The USGS values for these layers are typically one order of magnitude lower than the values in the TSPA-93 data set.

The decreased alphas mean that these formations would have generally higher capillary pressures and saturations than would be expected from the TSPA values.

Almost all of the USGS van Genuchten m values are less than the TSPA-93 values, which indicates that the USGS moisture retention analyses resulted in capillary pressure-saturation curves with distinctly different characteristics than the TSPA-93 analyses. The USGS results indicate that the matrix samples were found to have pore-size distributions that are broader than those measured in the TSPA-93 analyses.

3.2.2.2 Fracture Properties

Fracture parameters are available from theoretical analyses and saturated zone tests (TSPA-93), direct measurements of in-situ air permeability (USGS), and the results of pneumatic data analyses (LBNL with USGS data). The theoretical analysis described in TSPA-93 developed representative fracture porosities and van Genuchten parameters for the hydrogeologic units. This parameter set has been used in many Yucca Mountain modeling studies. LeCain and Walker (1994) and Rousseau et al. (1996) of the USGS have reported air permeability (air- k) values for the various geological formations at Yucca Mountain.

Additional fracture permeability estimates have been developed at LBNL by Ahlers et al. (1996) using pneumatic borehole data from J. Rousseau of the USGS. The estimates were obtained by using submodels of the UZ model to determine pneumatic diffusivities for various geologic formations. The diffusivities were converted to permeabilities using an estimate of the composite porosity of the fractures and surrounding matrix which affect the diffusivities. Table 3.2.2-3 provides a summary of the fracture permeability estimates available from various sources.

The fracture permeabilities estimated using the Q pneumatic data are concluded to be the best values for the model calibration effort for most of the layers because they are representative of larger volumes than the air- k testing. Where fracture permeability estimates were available from several borehole pneumatic data sets, the geometric mean of a layer was calculated and used as an initial estimate in the model calibration. There is little attenuation of the atmospheric signal through the geologic formations which comprise the highly fractured TCw and TSw, so that there is only one mean value of fracture permeability which is applicable to all of the layers within those hydrogeologic units. Additionally, few fracture permeability estimates were available for the layers below the TSw from the pneumatic data. Because of this, the permeability estimate calculated by Ho et al. (1995) based on TSPA-93 data was used for the zeolitic layers in the CHn.

These mean values calculated from Ahlers et al. (1996) results are consistent with the data reported by LeCain and Walker in their air- k testing. The values

Saturation and Capillary Pressure Analysis

Table 3.2.2-3
Fracture Permeability Estimates

TSPA-93		USGS Mean Air-k values (Rousseau et al., 1996)	LBNL Permeability Estimates (Ahlers et al., 1996)	
Unit	(m ²)	(m ²)	(m ²)	Layer
1	4.1E-9	NA	5.8E-12 ²	Upper Tpcpxxx
1	4.1E-9	(1.3 to 25.7) E-12	5.8E-12 ²	Middle Tpcpxxx
1	4.1E-9	NA	5.8E-12	Tpcpv3,2
3c	4.6E-9	NA	4.0E-12 ³	Tprv2,1
3c	4.6E-9	(0.2 to 2.2) E-12	4.0E-12 ³	Tptrn
3c	4.6E-9	(0.3 to 4.1) E-12	4.0E-12 ³	Tptrl, Tptpul
3r	4.6E-9	(0.6 to 1.1) E-12	4.0E-12 ³	Tptpmn
3r	4.6E-9	0.4 E-12	4.0E-12 ³	Tptpll
3r	4.6E-9	~2 E-12 ¹	4.0E-12 ³	Tptpln
4	5.3E-9	NA	1.0E-11	Tptpv3
6	1.9E-9	NA	1.0E-13 ⁴	Tptpv2,1, Tpbtl(z)
6	1.9E-9	~3 E-14 ¹	1.0E-13 ²	Ta(z)
6	1.9E-9	NA	1.0E-13 ²	Thbt, Prow Un. 4 (z)
7	1.3E-8	NA	3.0E-14	Prow Un. 3
6	1.9E-9	NA	1.0E-13 ²	Prow Un. 2,1; Tcbtl(z)
5	6.5E-9	NA	3.0E-14 ²	Tptpv2, 1, Tpbtl
5	6.5E-9	NA	3.0E-14 ²	Ta

¹Preliminary data from UZ#16 borehole air-k testing, personal communication, G. LeCain, USGS, July, 1996. Provided for comparison purposes only.
²Assigned fracture permeability based on estimate for layer with similar properties.
³Analysis resulted in one estimate for entire unit.
⁴Estimated zeolitic fracture permeability based on arithmetic average of TSPA93 data set per Ho et al., 1995.

are also consistent with the preliminary estimates reported by Anna (1996) from his saturated fracture system modeling of the TCw.

All of the sublayers in the model were assumed to have fractures except the PTn. For the PTn, Q fracture data from ESF observations (Rousseau et al., 1996), corroborated by the results of non-Q pavement studies (Sweetkind et al., 1996), show that there are very few fractures that are connected across all of the PTn layers. The bedded units, in particular, prevent the propagation of fractures. However, the non-Q observations of bomb-pulse Cl-36 in the ESF (Fabryka-Martin et al., 1996) indicate the presence of fast-pathways across the PTn. Due to the spatial variability of these observations and their association with observed structural features, it is concluded that these pathways are localized. Therefore, they are not evidence of through-going fractures prevalent across the entire PTn.

3.3 Calibration Methodology

3.3.1 Development of Submodel

This section describes the development of a numerical model which will be used to simulate the hydrologic conditions established by the saturation and capillary pressure data. Since the objective of this study is to determine model-related parameters, ideally the full 3-D UZ model would be used in the calibration effort. However, inverse modeling requires solving the forward problem many times, rendering direct calibration of the UZ model computationally very inefficient. Furthermore, fracture and fault properties are not well known at this time and the assumed properties used in the 3-D model may have a significant effect on the flow patterns and resultant saturations and capillary pressures. Therefore, the calibration will be done with a set of 1-D columns taken from the 3-D UZ model. The columns are obtained from the nodes that correspond to the location of the borehole in the numerical grid representing the Yucca Mountain UZ.

3.3.2 Conceptual Model

The conceptual model used during the calibration presented in this chapter is based on a number of assumptions. The assumptions include the following:

1. *Steady-state condition and constant infiltration rates.* Saturation and capillary pressure data represent the hydrologic state of the UZ under steady state conditions and constant infiltration rates. Changes in net infiltration are expected to occur gradually over thousands of years due to climate changes. The permeabilities of some matrix layers in the TCw and TSw are as low as $1\text{E-}18\text{ m}^2$, and a Darcy Velocity of 0.3 mm/yr under a unit gradient is estimated for those layers. The relatively slow travel time makes saturation and moisture tension changes occur over long time periods. Therefore, infiltration pulses are dampened with depth, as shown a study by Wang and Narasimhan (1985). It should be emphasized that the presence of bomb-pulse isotopes is not necessarily an indication of high average infiltration rates, but that infiltration pulses of sufficient local intensity and duration to travel through the PTn and penetrate down to the proposed repository level in the TSw can occur.
2. *Uniform Infiltration Rates.* The infiltration rate was assumed to be uniform across the submodel domain during initial calibration runs. There is evidence that infiltration is spatially variable across the site (Flint et al., 1996); however, the range of rate estimates available from the project adds more uncertainties to the calibration. The runs to develop effective model layer parameters used a range of uniform rates to minimize this uncertainty. Therefore, the result of the calibration was a range of parameters. The uniform rate assumption was investigated by sensitivity studies using spatially variable infiltration rates.

3. *Validity of the Equivalent Continuum Model (ECM) approximation.* The ECM approximation (see Chapter 4, Wu et al., 1996) consists of the assumption that capillary pressures in the matrix are equal to capillary pressures in the fractures in an equivalent continuum system. This is true under steady-state conditions. Another consequence of the steady-state condition is that a model using the ECM will provide the same results as a dual-k model (Chapter 6, Doughty et al., 1996).
4. *Validity of the van Genuchten model.* This model has commonly been used on the project during simulation studies. A detailed study of its applicability to Yucca Mountain volcanic tuffs has not been done. However, the USGS presently has an apparatus to measure tuff relative permeability curves (D. Hudson, USGS, personal communication, April, 1996). If they can generate a number of curves, perhaps this assumption can be re-evaluated.

The relatively slow moisture travel times through the geologic layers discussed above makes it possible that saturations at depth within the mountain actually are a reflection of historic conditions with much different infiltration rates. Studies of historic infiltration rates and climate conditions show that the infiltration rate has varied widely. For instance, the past 10 years have been the wettest of the available record, with much of the infiltration contributed by only a few major storms. Mitigating this effect to some extent is the redistribution of moisture through spreading and evaporation into the air moving through the mountain due to barometric pumping (Weeks, 1987).

The recent measurements of bomb-pulse isotopes in the ESF (Fabryka-Martin et al. 1996) suggest that significant pulses of water can penetrate deep within the TSw through fracture flow. This flow would be characterized by episodic, transient events. However, the fracture surfaces encountered in the subsurface at Yucca Mountain are coated with deposits of calcite and other minerals (Paces et al., 1996). These fracture coatings have been found to sometimes reduce imbibition into the matrix significantly (Thoma et al., 1992).

This phenomenon and others such as fingering have been used to significantly reduce the amount of surface area interaction allowed between the fractures and the adjacent matrix in modeling studies using the dual permeability formulation (Ho et al., 1995) in order to achieve reasonable fracture flow travel times. In this case, fracture-matrix interaction is minimized, and even if there are infiltration pulses occurring in localized fracture networks, the conditions in the matrix may not be significantly affected. Bulk measurements (field or lab) are unlikely to detect such flow fast pathways and so the use of the data to calibrate a steady-state model is validated.

The steady-state assumption was used in the previous calibration effort (Ahlers et al., 1995) and resulted in a fairly good match of the observed data. The ECM approximation presently used in the UZ model has been changed

from the formulation used in the studies discussed in Ahlers et al. (1995) as presented in Chapter 4 (Wu et al., 1996) of this report. The present formulation allows for significant fracture flow, if warranted, at matrix saturations significantly less than 1. Fracture and matrix saturations and capillary pressures and thus flows are separately controlled by assuming that the distribution of fractures in each model layer can be simulated with a representative set of parameters, including van Genuchten coefficients, permeability, porosity, and residual saturation. The fracture and matrix parameters can be independently adjusted so that fracture flows across each layer can match travel times estimated from isotope data while maintaining capillary pressure equilibrium. This, of course, allows small quantities of moisture to travel down through the fractures, but the bulk of the flow is in the matrix.

Using a range of infiltration rates in the calibration will cause the resultant parameter sets to vary. In particular, as the infiltration rate is increased, matrix permeabilities should increase so that the matrix can conduct more water without increasing saturations or changing capillary pressures. At the same time, the fractures should conduct more water, increasing saturations and reducing capillary pressures in the fractures. The fracture alpha parameter will then have to decrease in order to continue to match the matrix capillary pressures at a higher fracture saturation.

3.3.3 Inversion Code and Formulating the Inverse Problem

The calibration effort involved using numeric grids from the 3-D site-scale model and calibrating the hydrogeological parameters used in the grids against the measured saturation and capillary pressure data. The inversion code which performed the calibration was the ITOUGH2 program (Finsterle, 1993). It offers a sophisticated tool for performing inversions against measured data. This code is qualified under the LBNL QA program. A detailed explanation of the methodology used in ITOUGH2 is provided in Finsterle (1993).

The inverse problem for this calibration consists of estimating effective hydrogeologic parameters by simultaneously matching the available saturation and capillary pressure data from the boreholes listed in Table 3.2.1-1. The goodness of fit of the calibration is measured using the standard least squares approach to minimize the sum of the squared weighted residuals. There are two types of residuals. The first type consists of the differences between the observed and calculated variables representing the system state (saturations and capillary pressures). The second type consists of the differences between the initial parameter estimates used as input to the inversion and the resultant calibrated parameters. All residuals are weighted by the reciprocals of the assigned standard deviations. The standard deviations for the saturations, capillary pressures, and parameter estimates are a reflection of the expected match between the data and the predictions from the calibrated model.

3.3.4 Parameter Sensitivity Selection

The measure of the sensitivity of each parameter calculated by the program is based on the Jacobian matrix filled with the sensitivity coefficients (which are the partial derivatives of the residuals with respect to the parameters included in the inversion). The measure is the sum of the sensitivity coefficients of all observations with respect to the parameter of interest, scaled by the expected variation of the parameter and by the inverse of the standard deviation of the observations (Ahlers et al., 1995).

Selecting parameters that are subjected to the inversion process involves choosing those that have a significant effect on the simulation results for the saturations and capillary pressures. Preliminary runs with the program showed that many of the permeability and van Genuchten model fitting coefficients for the matrix and fractures were sensitive; i.e., that small changes in parameter values had a relatively significant effect on the results. The residual saturation values for the matrix and fractures, however, were found to be relatively insensitive, and were omitted from subsequent inversion runs.

As ITOUGH2 attempts to converge to a parameter set that minimizes the residuals between the observed and simulated data, it varies the parameters to different degrees to provide the best fit. In fact, if the program finds that a parameter is insensitive, it may vary it widely in trying to achieve a better fit. If allowed to do this, ITOUGH2 may converge to a parameter set which fits the data well but is very different from the initial parameter estimates.

Since the initial parameter estimates to the calibration are based on numerous physical measurements, an approach that preserved as much of the initial information as possible consists of limiting the ability of ITOUGH2 to vary insensitive parameters. First the program determines the sensitivity of the parameters, and varies only those parameters above a preset limit. The limit is found by performing several preliminary inversions with different limits and evaluating how many parameters are being varied during the inversion. If the parameter sensitivity is found to be smaller than the pre-set limit, the parameter is temporarily not used in attempting to improve the fit. Since the sensitivity coefficients change during the optimization process as parameters are adjusted, the sensitivity evaluation is repeated every few iterations to make sure that parameters becoming sensitive due to changes in the parameter set are not omitted from the inversion. In this way, inactive parameters may become active and vice versa during the inversion.

3.3.5 Formulation of Submodel and Calibration Methodology

The primary submodel used in the calibration effort was constructed by extracting from the UZ model all vertical columns corresponding to the borehole locations with available Q saturation and capillary pressure measurements. The submodel thus consists of a set of five 1-D pillars which are horizontally disconnected. This submodel shares discretization, zonation, and boundary conditions with the UZ model. Since the initial goal of the calibration

was to develop a set of effective parameter values for each layer, the individual columns had common parameter values for the rock properties representing model layers.

The resultant submodel for use in the calibration consisted of more than 20 model sublayers in each column, depending on the height of the column above the water table. Each sublayer had a set of initial estimate properties for the matrix and fractures, including a set of relative permeability and capillary pressure functions. This results in a large number of potential parameters to be estimated. Mishra et al. (1994), showed that saturation and capillary pressure at a given location depend primarily on the properties of the sublayer in which the sampling location lies, and only marginally on the properties of the adjacent layers. This fulfills the ITOUGH2 requirement of independent parameter estimation. However, it leads to a situation in which only a limited data set is available for the estimation of all hydrogeologic parameters of a certain layer because only data from that layer can be used in its calibration.

The boundary conditions for the 1-D columns are set as follows: at the top, the columns are at atmospheric conditions, and a constant temperature of 25 deg. C is applied. Pressure at the water table is held constant at about 92.7 kPa. An isothermal steady-state calculation is performed using the EOS3 module of TOUGH2 (Pruess, 1987; 1991). This code is qualified under the LBNL QA program.

One representative capillary pressure and saturation data point was provided for each model layer grid block. The data points were generated by arithmetically averaging the available core sample data obtained within a geologic layer and assigning the result to the corresponding model layer. Because of the averaging process, the scatter in the core sample data set is decreased.

All saturation or capillary pressure data used in the inversion are considered to be of comparable quality. Preliminary data from the USGS (Flint, 1996) indicated that the standard deviations of mean saturations of geologic layers measured from core samples ranged from 0.03 to 0.33. Based on this, a standard deviation of 0.10 was assigned to the saturation data. As the capillary pressures can vary over several orders of magnitude, especially in UZ-14, the inversion compared the logarithms of the capillary pressures. Preliminary data from Flint (1996) showed that for the geologic layer mean capillary pressures (ranging from 0.1 to a maximum of about 13.0 bars), the standard deviations were substantial. Because of this, a relatively large uncertainty of one order of magnitude was assigned to the potential data.

The parameter values used as input to the inversions were also weighted according to the preliminary data provided by Flint (1996). The concept of using prior information about the model parameters during the inversion was justified because the current values are based on extensive measurements. Since

they are not just initial guesses for the inverse modeling process, they were used as data points. Furthermore, only very limited data of the system state itself were available because the use of the UZ model grid provided one average data point of each type per layer. Therefore, the use of prior information in the parameter determination was imperative to reduce non-uniqueness and avoid instabilities. The standard deviations assigned to the prior information were obtained from the preliminary data provided by Flint (1996).

The methodology used in the calibration effort is summarized as follows:

1. Develop a set of 1-D columns from the 3-D model corresponding to the five borehole locations.
2. Use the 1-D columns in a combined run to determine effective parameters for a range of uniform infiltration rates and a set of variable rates from an infiltration map developed by the USGS.
3. Perform sensitivity analyses of the results by comparing the effective parameter set with the results from finely-gridded 1-D columns, different initial parameter sets, inversion methodologies, and coupling permeability and van Genuchten alpha parameters during other inversions.
4. Use the effective parameters in a forward run with the entire 3-D UZ model and compare the results with the 1-D column inversions.

3.4 *Combined Column Inversions, Uniform Infiltration Rates*

3.4.1 Uniform Infiltration Rates

The inversion during the prior calibration (Ahlers et al., 1995) investigated a single uniform infiltration rate in determining the best fit to the data. It also evaluated the uniform rate which would result in the best match to the measured data. Because of the uncertainties in the spatial variability and net quantity of infiltration as discussed above, this study was not limited to one uniform infiltration rate. A range of infiltration rates were investigated during separate inversions to evaluate the effect of rate increases on the resultant parameter set. This approach also provides an evaluation of the conceptual model. The uniform rates applied to each column during modeling included 0.01 mm/yr, 0.1 mm/yr, 1.0 mm/yr, and 5.0 mm/yr.

3.4.2 Combined Column Inversion Approach

The 1-D columns used in the inversion were obtained from the 3-D UZ model grid. The 3-D model grid represents vertical variations in the unsaturated zone with at least one model layer for each important geologic layer and altered zone as described in Chapter 1. Additional refinement is provided in the model layers associated with the proposed repository. One point of each data

type per model layer was calculated for the calibration as discussed above. The intent of these first runs was to develop sets of effective layer average values at each uniform infiltration rate. Subsequent runs then matched the borehole data sets for SD-7 and SD-9 individually to evaluate the spatial variability in parameters.

Given the noise of the data, the selection of the calibration points was done by averaging all of the data across the geologic layer corresponding to model layer. In the combined run, data from different boreholes contribute to the calibration of an effective parameter in one model sublayer. For shallow geologic formations penetrated by a number of boreholes, this results in a match of a horizontally-averaged system behavior. For deeper geologic layers that are reached by only a few boreholes, fewer data points exist for the calibration and the uncertainty of the result is greater. The same initial parameter estimates were used as the input to the inversions at the different infiltration rates. This preserved as much of the prior information from the permeability estimates as possible, and prevented the results from being biased by different initial estimates. Different initial estimates and their associated standard deviations present a different problem for the inversion to solve.

3.4.3 Combined Column Results, 0.1 mm/yr Uniform Infiltration Rate

The matches for the boreholes used in the combined columns with a uniform infiltration rate of 0.1 mm/yr are shown in Figures 3.4.3-1 through -4. Looking at the profiles, it is important to recall that a simultaneous inversion was done with all the 1-D columns using available data. It was not the goal of this combined column inversion to match individual saturation profiles, but to come up with a consistent parameter set that best reproduces the overall system behavior at Yucca Mountain using the site-scale model. This means that there is the possibility that certain profiles or portions of profiles may actually be matched worse after calibration, but the calibration approach ensures that the overall performance of the model has improved. Also, as discussed previously, the layer-average values smooth out the peaks in the core sample data to some extent. Therefore, the matches are evaluated with respect to the layer average-values and not the peaks in the core sample data.

Saturation and Capillary Pressure Analysis

Figure 3.4.3-1
Liquid Saturation and Capillary Pressure for Borehole SD-7. Core sample data from L. Flint, USGS.

Figure 3.4.3-2
Liquid Saturation and Capillary Pressure for Borehole SD-9. Core sample data from L. Flint, USGS.

Saturation and Capillary Pressure Analysis

Figure 3.4.3-3
Liquid Saturation and Capillary Pressure for Borehole UZ-14. Core sample data from L. Flint, USGS.

Figure 3.4.3-4
Liquid Saturation Profiles for Boreholes SD-12 and UZ#16. Core sample data from L. Flint, USGS.

The saturation and capillary pressure plots for borehole SD-7 in Figure 3.4.3-1 present the core sample data from the USGS, calculated layer-average data, pre- and post-calibration profiles, and location of hydrogeologic unit boundaries. The absolute value of the capillary pressures are used to allow the use of a log-scale in the plot. The profiles show that the measured data were matched fairly well by the calculated saturations from the initial estimate parameters before calibration. However, the fit was improved somewhat after calibration, especially in the upper layers of the TSw.

The fit is better for the saturation than for the capillary pressure because the capillary pressure core data are too variable to be matched during the inversion. The data can vary more than two orders of magnitude in one geologic layer. However, the trends in the capillary pressure are followed in the profile. The profile dips slightly towards the lower measurement limit of 0.1 bars in the vicinity of the perched water location in the CHn. The layer-average point shown in this location was added to the capillary pressure data because of the known presence of perched water, even though no potential measurements were reported at this elevation.

Similar results are obtained for borehole SD-9 shown in Figure 3.4.3-2. The calibration does not provide a good match of the decrease in saturation which occurs at the boundary of the TSw/CHn hydrogeologic units. This occurs because the first model layer of the CHn below the boundary is partially vitric and partially zeolitic. For the modeling purposes, the layer was assigned zeolitic properties in order to capture the effect of the alteration on permeabilities and moisture flow. Because of this, the vitric peak in the area was not captured well. The low saturation peak in the Prow Pass Unit 3 below the CHn was matched well, however.

Capillary pressures for borehole UZ-14 shown in Figure 3.4.3-3 were the driest reported for the three boreholes. Therefore, the capillary pressure data were not matched well by the calibrated parameter set. In-situ borehole measurements of capillary pressures in the nearby borehole UZ-1 have been compared to core sample values by Rousseau et al. (1996). The comparison shows that the in-situ values are all less than 10 bars, even though the cores show many measurements greater than 10 bars. However, saturations show a good match, especially in the zeolitic CHn and Prow Pass Unit 3. There are no capillary pressure measurements for boreholes SD-12 and UZ#16 shown in Figure 3.4.3-4. However, the saturation profiles show approximately the same match as the other boreholes.

For borehole SD-12, however, the properties assigned to the top CHn model layer in the pre-calibration run were assumed to be vitric on the basis of borehole log reports. However, the average saturation in the layer is about 85%, and a review of the mineralogic log showed that the tuff material is about 50% altered. Therefore, the layer was assigned zeolitic properties during the calibra-

tion run which results in the large difference between the initial and final conditions. For UZ#16, the saturation decrease in the Prow Pass Unit 3 is slightly less than expected from the layer average value, most likely because the presence of the adjacent water table boundary condition maintains a high saturation in the model layer.

3.4.3.1 Statistical Analysis and Parameter Sensitivity

The fit between the observed and calculated saturations and capillary pressures must be assessed before the calibrated parameter set can be evaluated. If the match is not improved by the calibration, the parameter estimates cannot be considered representative for Yucca Mountain. However, in this inversion the fits of the saturation and capillary pressure data were improved.

As discussed previously, ITOUGH2 attempts to minimize the weighted sum of squared residuals of the simulation results from the measured data. If the resultant residuals are close to zero, it indicates that the average system behavior has been well-reproduced. A simple way to characterize the residual set is to calculate its standard deviation. A small standard deviation means that the residuals are relatively tightly clustered, while a larger deviation means that the set is less tightly grouped. Obviously a smaller residual standard deviation (RSD) is representative of a better match to the measured data.

Another measure of the fit is the bias of the measured data as compared to calculated data. The bias is the sum of the residuals from the data set. For example, if the saturation bias is determined to be zero, it would mean that the inversion resulted in a calculated data set where the sum of the residuals due to points drier than the measured data equaled the sum of the residuals from the points wetter than the measured data. This would be the optimum situation. It is possible to have 0 bias but a very large RSD.

Table 3.4.3-1 presents a summary of the residual standard deviations (RSDs) and biases for the uncalibrated and calibrated saturation and capillary pressure data sets. As discussed above, the inversion matched the logarithms of the capillary pressure data. Therefore, the results for the capillary pressure data set are presented in terms of logarithms. It also presents a summary of the reduction in the sum of squared weighted residuals for the set of saturation and capillary pressure data during the inversion.

Saturation and Capillary Pressure Analysis

Table 3.4.3-1 0.1 mm/yr Rate Residual Standard Deviation (RSD) and Bias Summary				
Data Set Results				
		Uncalibrated	Calibrated	
Datatype	RSD	Bias	RSD	Bias
Saturation	0.13	-0.05	0.09	-0.01
log (Cap. Press.)	0.72	-0.08	0.66	-0.05
SSWRD ¹	206		113	
¹ SSWRD= sum of squared weighted residuals				

A statistical analysis of the set of residuals from the 0.1 mm/yr uniform infiltration rate shows that the standard deviations of the saturation was reduced from 0.13 to 0.09 by the calibration effort. The RSD for the capillary pressure match was reduced from 0.72 to 0.66, but the analysis shows that the bias of the initial estimate was rather small. This indicates that the measured capillary pressure data are widely scattered and that the fit provided by the initial estimate set was almost as good as that achieved by the calibrated set. The inversion resulted in a reduction of the initial value of the sum of the squared weighted residuals of 206 to a value of 113.

Figure 3.4.3-5

Model Layer Parameter Sensitivity. 0.1 mm/yr uniform infiltration rate inversion. Overall sensitivity of the parameters in each layer to the liquid saturation and capillary pressure data during the inversion.

As discussed above, the overall sensitivity of a parameter is the sum of the absolute sensitivity coefficients (which are the partial derivatives of the residuals with respect to the parameters included in the inversion), scaled by the expected variation of the parameter and by the inverse of the standard deviation of the observation. Figure 3.4.3-5 shows a plot of the overall sensitivities of the parameters used in the inversion at the 0.1 mm/yr infiltration rate. The plot shows that the van Genuchten m values are not sensitive and so do not contribute towards improving the fit. Conversely, van Genuchten m values cannot be determined from the available saturation and capillary pressure data. Fracture permeability and matrix van Genuchten α values show limited sensitivities, with some exceptions. Fracture permeabilities sensitivities are relatively high for the tsw33 and the ch3zc, while matrix alphas are elevated for tsw31 and tsw35. The matrix permeability is sensitive in layers ptn23, tws31, tsw35, and pp3vp. This parameter shows the most sensitivity at this infatuation rate.

Figure 3.4.3-6
Liquid saturation sensitivity coefficients with respect to matrix permeability and fracture alpha of layer tsw31 vs. Elevation for borehole SD-7. 0.1 mm/yr uniform infiltration rate inversion.

Model parameters can only be determined if the calculated saturations and capillary pressures at a measurement point are sensitive with respect to changes of these parameters. As an example, Figure 3.4.3-6 shows the sensitivity coefficients of calculated saturations at borehole SD-7 with respect to the matrix permeability and fracture alpha of layer tsw31. Layer tsw31 displayed the highest overall sensitivity to the data as discussed above.

The plot shows that the saturation in layer tsw31 is the most sensitive to the matrix permeability in tsw31, as expected. Liquid saturations in the layers above layer tsw31 are somewhat less sensitive to the tsw31 matrix permeability and resultant saturation depending on their elevation above tsw31. However, saturations in the layers below tsw31 are not sensitive to conditions in tsw31. The fracture alpha sensitivity coefficients are all very small, with just a slight increase in and above layer tsw31. This means that the calculated saturations in the model layers are not affected by changes in the fracture alpha for tsw31. This is expected in cases such as this when the matrix permeability values are greater than the flux of 0.1 mm/yr.

ITOUGH2 provides extensive information about the uncertainties of the resultant parameter sets. The parameter set for the 0.1 mm/yr inversion has been evaluated for both the conditional and joint standard deviations (CSD and JSD) of the estimated parameters. The CSD gives an estimate of the uncertainty of the parameter provided that all the other parameters are fixed. The JSD takes into account correlations with other parameters and their uncertainties, and is always greater than or equal to the conditional estimate. The CSDs of the permeability data set, for example, average about two orders of magnitude. This indicates that the saturation and capillary pressure data do not contain enough information for a unique and independent determination of hydrogeologic parameters. Changing parameters by their respective standard deviations still leads to an acceptable match of the data. So, although the fits to the data from the calibrated data set are reasonable, the uncertainty associated with any given parameter is large.

Figure 3.4.3-7

Normalized Standard Deviations (NSD) of Parameter Estimates for Model Layers, 0.1 mm/yr inversion. (NSD= conditional standard deviation/ parameter value)

Figure 3.4.3-7 presents CSDs normalized by dividing them by the parameter estimates to provide a relative comparison of uncertainties for the parameter set. The log values of the permeability and alpha estimates were used in this calculation. The data show several peaks in the matrix permeability uncertainty plot in layers ptn22 and ch1zc corresponding to the Tpy and zeolitic Tptpv1 and Tpbtl, respectively. These peaks correspond to layers where the calibration data varied significantly. The matrix alpha and m parameter standard deviations are more consistent and relatively low across the model layers.

The fracture alpha and m parameters show large standard deviations with very few exceptions. The exceptions occurred in layers such as tw11 and tsw33 with very low estimated matrix permeabilities. A review of Figure 3.4.3-5 shows that the sensitivities of the fracture alpha and m parameters were relatively high compared to those of other layers, especially in layer tsw33. Because of this sensitivity, the inversion resulted in an estimate with a relatively small uncertainty. The fracture alpha and m SDs in the other layers are high because the sensitivities were low, preventing the inversion from providing more constrained estimates. The reason the high SDs for the fracture alpha values are so consistent is that they were all assigned the same large a priori standard deviation as initial

Saturation and Capillary Pressure Analysis

estimates to the inversion. As discussed above, the fracture alphas are theoretical values obtained from the TSPA-93 and their applicability to the complex fracture networks at Yucca Mountain is not clear.

3.4.4 Combined Column Results, All Uniform Infiltration Rates

The same initial parameter set was used for each of the uniform infiltration rate inversions so that the inverse problems posed to ITOUGH2 were consistent. Some statistical results for the runs are shown in Table 3.4.4-1. Similar to the 0.1 mm/yr case, the table provides the standard deviation of the set of differences between the calculated and measured saturation and capillary pressure data. It also provides the bias of the resultant predictions and the reduction in the sum of the squared and weighted residuals during the inversions.

Table 3.4.4-1 Residual Standard Deviation (RSD) and Bias Summary				
Datatype/Rate	Run			
	Uncalibrated		Calibrated	
	RSD	Bias	RSD	Bias
0.01 mm/yr				
Saturation	0.13	0.03	0.08	-0.01
log (Cap. Pres.)	0.82	-0.37	0.67	-0.05
SSWRD ¹	222		108	
0.1 mm/yr				
Saturation	0.13	-0.05	0.09	-0.01
log (Cap. Pres.)	0.72	-0.08	0.66	-0.05
SSWRD	206		113	
1.0 mm/yr				
Saturation	0.18	-0.12	0.09	-0.02
log (Cap. Pres.)	0.88	0.38	0.66	0.01
SSWRD	377		113	
5.0 mm/yr				
Saturation	0.21	-0.16	0.10	-0.05
log (Cap. Pres.)	1.22	0.79	0.67	0.16
SSWRD	547		136	
¹ SSWRD= sum of squared weighted residuals				

As the table shows, the 0.1 mm/yr inversion had the smallest residual standard deviations (RSD) for the uncalibrated parameter set. The capillary pressure bias is very low compared to the other uncalibrated runs, and the saturation bias relatively low. The smallest saturation bias in an uncalibrated run is from the 0.01 mm/yr inversion. The uncalibrated runs at the higher rates predicted saturations much higher than the measured data as shown by the larger saturation biases. This results in much higher RSDs for the uncalibrated runs.

The calibration reduced the RSDs and biases of the saturation and capillary pressure residual sets at all infiltration rates. The best calibrated fits based on the bias and RSD results were achieved for the uniform infiltration rate of 0.01 mm/yr. However, the range of saturation RSDs of 0.08 to 0.10 between the various calibrated runs is too small to be significant. After calibration, the fit of the capillary pressure log data was about the same for all of the inversions, or about 0.67 of a log cycle. This relatively large residual standard deviation from the calibrated parameter set is the result of the scatter in the original capillary pressure data set. Due to this scatter, the calibration could only improve the fit to an RSD of 0.67 of a log cycle at all infiltration rates.

The increase in the absolute values of the biases and RSDs with increasing infiltration rate may be an indication that the steady-state conditions assumed for the higher infiltration rates is unrealistic. If the net rate is similar to one of the higher rates used in this study, it is possible that much of the additional flux is due to extreme storm events contributing pulsed flow through localized structural features. Alternatively, it might be an indication that the uniform rate assumption for all boreholes at these higher fluxes is unrealistic, especially since a number of spatially variable infiltration maps have been developed for the project which show that the infiltration rate is not uniform.

Figure 3.4.4-1
Liquid Saturation and Capillary Pressure for Borehole SD-7 at Various Infiltration Rates.
Core data from L. Flint, USGS.

Figure 3.4.4-1 shows the results of the calibrations done at different infiltration rates for borehole SD-7. The plot shows that as the infiltration rate increases, the simulated saturations increase and the simulated capillary pres-

Saturation and Capillary Pressure Analysis

asures decrease toward the experimental measurement limit of 0.1 bars as previously seen in the bias and RSD data presented above. Similar behavior can be seen in profiles for the other boreholes used in the inversion and so are not presented here.

As the infiltration rate increases by 2.5 orders of magnitude from the initial rate of 0.01 mm/yr, the hydrogeologic parameters of the model are adjusted during the inversion to match the observed data. A summary of the resultant model parameters are provided in Table 3.4.4-2.

Table 3.4.4-2 Summary of Calibrated Uniform Rate Model Parameters					
Layer Designation (Buesch et al., 1995)	Prior Data	Infiltration Rate			
Matrix Permeability (m ²)		0.01 mm/yr	0.1 mm/yr	1.0 mm/yr	5.0 mm/yr
Upper Tpcxxx	1.5E-19	1.60E-19	1.60E-19	1.60E-19	1.60E-19
Middle Tpcpxxx	5.4E-18	1.36E-17	3.41E-17	2.15E-16	5.40E-18
Tpcpv3,2	2.2E-17	2.20E-17	2.20E-17	2.20E-17	2.20E-17
Tpcpv1,Tpbt4	4.0E-13	4.00E-13	4.00E-13	4.00E-13	4.00E-13
Tpy	3.0E-16	2.40E-13	2.40E-13	2.40E-13	2.40E-13
Tpbt3	5.2E-14	4.50E-16	7.55E-15	5.03E-14	2.04E-13
Tpp	8.8E-14	8.80E-14	8.80E-14	4.08E-14	2.21E-13
Tpbt2,Tptrv3	4.2E-13	4.20E-13	3.11E-13	1.11E-12	2.25E-12
Tptrv2,1	1.6E-16	1.60E-16	2.54E-15	1.01E-13	2.04E-13
Tptm	1.7E-16	4.30E-16	6.77E-15	7.41E-14	2.57E-13
Tptrl,Tptpul	2.0E-17	5.02E-19	2.15E-18	3.17E-18	2.00E-17
Tptpmn	4.0E-18	4.00E-18	2.52E-17	4.00E-16	4.00E-18
Tptpll	2.3E-17	3.21E-19	3.34E-17	2.86E-16	9.16E-18
Tptpln	9.6E-17	9.60E-17	9.60E-17	9.60E-17	3.13E-16
Tptpv3	5.0E-18	2.00E-17	2.00E-17	1.26E-16	7.96E-16
Tptpv2,1,Tpbt1(z)	5.4E-16	5.40E-16	5.40E-16	5.40E-16	5.40E-16
Ta(z)	4.5E-18	4.50E-20	7.13E-19	4.50E-18	4.50E-18
Thbt, Prow Un. 4 (z)	8.4E-18	8.40E-18	8.40E-18	8.40E-18	5.30E-17
Prow Un. 3	3.8E-17	2.97E-17	5.22E-16	3.50E-15	1.69E-14
Prow Un. 2,1,Tcpbt(z)	1.7E-17	1.70E-17	1.70E-17	4.27E-17	2.69E-16
Tptpv2,1,Tpbt1	1.6E-12	1.60E-12	1.60E-12	1.60E-12	1.60E-12
Ta	5.5E-14	5.50E-16	2.19E-14	5.50E-14	8.69E-14

Saturation and Capillary Pressure Analysis

Table 3.4.4-2 (cont.)
Summary of Calibrated Uniform Rate Model Parameters

Fracture Permeability (m ²)	Prior Data	0.01 mm/yr	0.1 mm/yr	1.0 mm/yr	5.0 mm/yr
Upper Tpcxxx	5.8E-12	4.38E-12	6.01E-12	6.36E-12	8.38E-12
Middle Tpcpxxx	5.8E-12	5.75E-12	5.75E-12	5.75E-12	3.84E-11
Tpcpv3,2	5.8E-12	5.75E-12	5.75E-12	5.75E-12	5.75E-12
Tptrv2,1	4.0E-12	3.95E-12	4.00E-12	4.00E-12	4.00E-12
Tptm	4.0E-12	4.00E-12	1.00E-11	6.30E-12	3.47E-12
Tptl,Tptpul	4.0E-12	2.29E-12	6.30E-12	6.96E-12	8.37E-12
Tptpmn	4.0E-12	4.00E-12	4.00E-12	4.00E-12	1.59E-11
Tptpl	4.0E-12	8.73E-12	4.00E-12	4.00E-12	1.04E-11
Tptpln	4.0E-12	4.00E-12	4.00E-12	4.00E-12	4.00E-12
Tptpv3	1.0E-11	4.00E-12	4.00E-12	4.00E-12	4.00E-12
Tptpv2,1,Tpbt1(z)	1.0E-13	1.00E-13	1.00E-13	1.00E-13	1.00E-13
Ta(z)	1.0E-13	5.99E-14	1.00E-13	1.00E-13	1.00E-13
Thbt, Prow Un. 4 (z)	1.0E-13	1.00E-13	1.00E-13	1.00E-13	1.00E-13
Prow Un. 3	3.0E-14	3.00E-14	3.00E-14	3.00E-14	3.00E-14
Prow Un. 2,1,Tcpbt(z)	1.0E-13	1.00E-13	1.00E-13	1.00E-13	1.00E-13
Tptpv2,1,Tpbt1	3.0E-14	7.23E-13	7.23E-13	7.23E-13	7.23E-13
Ta	3.0E-14	7.23E-13	7.23E-13	7.23E-13	7.23E-13
Matrix van Genuchten alpha (1/Pa)	Prior Data	0.01 mm/yr	0.1 mm/yr	1.0 mm/yr	5.0 mm/yr
Upper Tpcxxx	3.4E-06	1.55E-05	1.88E-05	1.56E-05	1.70E-05
Middle Tpcpxxx	1.2E-06	1.70E-06	1.32E-06	1.63E-06	1.28E-06
Tpcpv3,2	2.3E-07	1.17E-06	1.35E-06	6.48E-07	2.30E-07
Tpcpv1,Tpbt4	3.7E-05	2.13E-05	2.20E-05	2.51E-05	3.89E-05
Tpy	7.6E-06	9.87E-06	1.19E-05	1.40E-05	1.54E-05
Tpbt3	2.6E-05	3.59E-05	3.66E-05	4.20E-05	4.32E-05
Tpp	3.4E-05	2.15E-05	3.05E-05	3.41E-05	3.61E-05
Tpbt2,Tptrv3	9.8E-05	1.52E-04	1.84E-04	1.68E-04	1.95E-04
Tptrv2,1	3.4E-06	3.41E-05	2.58E-05	2.66E-05	2.66E-05
Tptm	2.0E-05	1.91E-05	1.81E-05	1.93E-05	2.24E-05
Tptl,Tptpul	6.6E-06	6.01E-06	6.60E-06	6.70E-06	5.48E-06
Tptpmn	6.4E-07	8.44E-07	8.02E-07	8.12E-07	8.53E-07
Tptpl	2.7E-06	3.35E-06	3.50E-06	3.02E-06	3.13E-06
Tptpln	4.7E-07	5.56E-07	5.62E-07	5.17E-07	5.21E-07
Tptpv3	1.0E-07	1.76E-06	1.12E-06	1.09E-06	7.98E-07
Tptpv2,1,Tpbt1(z)	1.9E-07	4.87E-07	1.90E-07	1.90E-07	1.90E-07
Ta(z)	3.9E-06	4.80E-06	5.18E-06	5.25E-06	3.94E-06

Saturation and Capillary Pressure Analysis

Table 3.4.4-2 (cont.) Summary of Calibrated Uniform Rate Model Parameters					
Tabt, Prow Un. 4 (z)	1.5E-07	1.50E-07	1.50E-07	1.50E-07	1.50E-07
Prow Un. 3	1.8E-05	2.05E-05	2.06E-05	2.07E-05	1.93E-05
Prow Un. 2,1,Tcpbt(z)	1.8E-06	1.48E-06	1.79E-06	1.44E-06	1.79E-06
Tptpv2,1,Tpbt1	9.8E-05	6.29E-05	8.96E-05	8.65E-05	7.64E-05
Ta	9.8E-05	6.21E-05	7.16E-05	8.22E-05	8.80E-05
Frac. van Genuchten alpha (1/Pa)	Prior Data	0.01 mm/yr	0.1 mm/yr	1.0 mm/yr	5.0 mm/yr
Upper Tpcxxx	1.2E-03	2.75E-03	1.55E-03	6.16E-04	4.88E-04
Middle Tpcpxxx	1.2E-03	1.23E-03	1.23E-03	1.10E-03	3.47E-04
Tpcpv3,2	1.2E-03	1.23E-03	1.23E-03	1.23E-03	1.23E-03
Tptrv2,1	1.2E-03	1.39E-03	1.37E-03	1.22E-03	1.09E-03
Tptrn	1.2E-03	1.22E-03	8.64E-04	9.69E-04	7.70E-04
Tptrl,Tptpul	1.2E-03	8.64E-04	5.45E-04	2.73E-04	1.53E-04
Tptpmn	1.2E-03	1.22E-03	1.22E-03	1.37E-03	1.22E-04
Tptpll	1.2E-03	8.15E-04	1.22E-03	1.09E-03	1.22E-04
Tptpln	1.2E-03	1.22E-03	1.22E-03	1.22E-03	1.22E-03
Tptpv3	1.2E-03	1.22E-03	1.22E-03	1.22E-03	1.22E-03
Tptpv2,1,Tpbt1(z)	7.3E-04	7.30E-04	7.30E-04	7.30E-04	7.30E-04
Ta(z)	7.3E-04	1.38E-03	7.30E-04	5.80E-04	4.11E-04
Tabt, Prow Un. 4 (z)	7.3E-04	7.30E-04	7.30E-04	7.30E-04	4.61E-04
Prow Un. 3	1.2E-03	1.22E-03	1.22E-03	1.22E-03	1.09E-03
Prow Un. 2,1,Tcpbt(z)	7.3E-04	7.30E-04	7.30E-04	7.30E-04	6.51E-04
Tptpv2,1,Tpbt1	1.2E-03	1.22E-03	1.22E-03	1.22E-03	1.22E-03
Ta	1.2E-03	1.22E-03	1.22E-03	1.22E-03	1.22E-03
Frac. van Genuchten m value	Prior Data	0.01 mm/yr	0.1 mm/yr	1.0 mm/yr	5.0 mm/yr
Upper Tpcxxx	0.20	0.22	0.23	0.21	0.21
Middle Tpcpxxx	0.23	0.23	0.23	0.22	0.22
Tpcpv3,2	0.44	0.44	0.44	0.44	0.44
Tptrv2,1	0.20	0.20	0.20	0.20	0.20
Tptrn	0.25	0.25	0.25	0.25	0.25
Tptrl,Tptpul	0.25	0.26	0.27	0.26	0.25
Tptpmn	0.32	0.32	0.32	0.34	0.30
Tptpll	0.23	0.25	0.23	0.21	0.26
Tptpln	0.42	0.42	0.42	0.42	0.42
Tptpv3	0.37	0.37	0.37	0.37	0.37
Tptpv2,1,Tpbt1(z)	0.36	0.36	0.36	0.36	0.36
Ta(z)	0.22	0.24	0.23	0.23	0.23

Saturation and Capillary Pressure Analysis

Table 3.4.4-2 (cont.)
Summary of Calibrated Uniform Rate Model Parameters

Tabt, Prow Un. 4 (z)	0.48	0.48	0.48	0.48	0.47
Prow Un. 3	0.31	0.31	0.31	0.31	0.31
Prow Un. 2,1,Tcpbt (z)	0.31	0.31	0.31	0.31	0.31
Tptpv2,1,Tpbt1	0.23	0.23	0.23	0.23	0.23
Ta	0.23	0.23	0.23	0.23	0.23
Matrix van Genuchten m value	Prior Data	0.01 mm/yr	0.1 mm/yr	1.0 mm/yr	5.0 mm/yr
Upper Tpcxxx	0.20	0.23	0.23	0.23	0.22
Middle Tpcpxxx	0.23	0.23	0.23	0.23	0.23
Tpcpv3,2	0.44	0.41	0.46	0.43	0.43
Tpcpv1,Tpbt4	0.22	0.22	0.22	0.22	0.21
Tpy	0.49	0.31	0.31	0.31	0.31
Tpbt3	0.24	0.23	0.24	0.24	0.24
Tpp	0.30	0.30	0.29	0.30	0.30
Tpbt2,Tptrv3	0.23	0.23	0.22	0.23	0.23
Tptrv2,1	0.20	0.21	0.21	0.21	0.21
Tptrn	0.25	0.25	0.25	0.25	0.25
Tptrl,Tptpul	0.25	0.25	0.25	0.25	0.25
Tptpmn	0.32	0.32	0.32	0.32	0.32
Tptpll	0.23	0.22	0.22	0.22	0.23
Tptpln	0.42	0.42	0.41	0.42	0.42
Tptpv3	0.37	0.37	0.37	0.37	0.37
Tptpv2,1,Tpbt1(z)	0.36	0.36	0.36	0.36	0.36
Ta(z)	0.22	0.22	0.23	0.23	0.22
Tabt, Prow Un. 4 (z)	0.48	0.48	0.48	0.48	0.48
Prow Un. 3	0.31	0.33	0.31	0.30	0.30
Prow Un. 2,1,Tcpbt(z)	0.31	0.31	0.31	0.31	0.31
Tptpv2,1,Tpbt1	0.23	0.21	0.22	0.22	0.22
Ta	0.23	0.22	0.22	0.22	0.22

Figure 3.4.4-2
Matrix Permeability Change for Uniform Rate Combined Column Inversions.

Figures 3.4.4-2 through -7 show the changes in calibrated parameters as the uniform infiltration rate is increased during the calibration study. The first point of each data series on the plots is the initial estimate used as input to the calibration. Figure 3.4.4-2 presents the change in matrix permeabilities with infiltration rate. The heavy dark lines correspond to welded and zeolitic units, while light gray lines correspond to the vitric portions of the CHn and the PTn. The correlation between the model layer designation shown on the legend and the geologic formation is provided in Chapter 1 of this report.

The plot shows that many of the initial permeability estimates used in the inversions were changed significantly by the 0.01 mm/yr calibration. One example occurred in model layer ptn22 (Tpy), which was increased more than two orders of magnitude and remained relatively constant over the rest of the infiltration rates. Other examples included the ptn23, ch2vc, tsw35, tsw33, and

ch3zc, with initial estimates of permeability that were decreased significantly at the 0.01 mm/yr rate and generally increased as the infiltration rate increased. Model layers tsw33 and tsw35 correspond to the upper and lower lithophysal layers in the TSw. Layers ptr23 and ch2vc correspond to the bedded tuff between Tpy and Tpp, and to the vitric portion of the Calico Hills Formation, respectively. Layer ch3zc is the altered portion of the Calico Hills Formation. The permeability in this layer was decreased by the inversion in order to match the saturations and capillary pressures in the perched water zones at Yucca Mountain.

In general, Figure 3.4.4-2 shows that permeabilities of the layers either remained relatively constant at the different infiltration rates or increased as the infiltration rate increased to keep the matrix from being saturated. Some exceptions occurred in layers tcw12, tsw34, and tsw35 as the infiltration rate is increased from 1.0 to 5.0 mm/yr. The sudden decrease in permeability estimates for these layers is associated with significant decreases in fracture alpha values (Figure 3.4.4-5) which would tend to remove water from the matrix. Therefore, the permeabilities were decreased in order to increase saturations and maintain good fits to the measured data.

Figure 3.4.4-3
Fracture Permeability Change for Uniform Rate Combined Column Inversions.

Figure 3.4.4-3 shows the variation in fracture permeability with infiltration rate. Since many of the initial estimates were identical and were not changed during the calibration runs, some of lines are overlain. The lines where this occurs are marked on the plot. The data show that the fracture permeabilities

were not highly sensitive during the inversions and thus were not varied. One exception to this was the ch2vc layer, corresponding to the vitric Calico Hills formation. The ch2vc permeability was increased by more than an order of magnitude during the 0.01 mm/yr run. The inversions at the other infiltration rates showed this same increase. For comparison, the matrix permeability for the ch2vc layer at the 0.01 mm/yr infiltration rate was estimated to be about $5.5\text{E-}16\text{ m}^2$. The increase is probably due to the fact that the matrix permeability had to be decreased at the low infiltration rate to match the measured saturation, while the fracture k had to be increased to decrease fracture saturations and equalize the capillary pressures between the matrix and the fractures in the steady-state run.

Figure 3.4.4-4
Matrix van Genuchten alpha Change for Uniform Rate Combined Column Inversions.

Figure 3.4.4-4 presents the changes in the matrix van Genuchten alpha parameters with infiltration rate. Many of the alpha parameters were not changed significantly from the initial estimates. Some exceptions are seen for the three layers in the TCw and layers tsw31 and tsw37 (TSw upper and lower

vitrophyres, respectively). The estimate for layer ch1zc was increased from the initial value in the inversion at the 0.01 mm/yr rate to decrease saturations at the low infiltration rate, but the results from the other inversions did not change from the initial estimate, indicating that the parameter was not found to be sensitive during the inversions.

Figure 3.4.4-5
Fracture van Genuchten alpha Change for Uniform Rate Combined Column Inversions.

Figure 3.4.4-5 presents the changes in the fracture van Genuchten alpha parameters with infiltration rate. More than half of the alpha parameters were decreased up to an order of magnitude to equalize capillary pressures as the infiltration rate increased. Layers tsw34 and tsw35 corresponding to the proposed repository horizon showed the largest decrease between runs at 1.0 and 5.0 mm/yr. The unaltered layers in the CHn and Prow Pass Tuff showed little or no variation, indicating that fracture flow is not a significant component of the total flow through the layer. Of the zeolitic layers, only the ch3zc showed a significant variation in alpha. This probably occurred because the matrix permeability is so low ($4.5E-20$ at 0.01 mm/yr) that as the infiltration rate increased alpha had to decrease to equalize capillary pressures.

Saturation and Capillary Pressure Analysis

Figure 3.4.4-6
Matrix van Genuchten m Change for Uniform Rate Combined Column Inversions.

Figure 3.4.4-7
Fracture van Genuchten m Change for Uniform Rate Combined Column Inversions.

Figures 3.4.4-6 and -7 present the variation of the van Genuchten m parameters with infiltration rate for the matrix and the fractures, respectively. The m values are relatively constant over the range of infiltration rates used in the study. One exception occurs for the matrix in layer ptn22. The m value shows a large decrease from the initial estimate at the 0.01 mm/yr rate, and then remains constant for the rest of the infiltration rates. The initial m estimate was the highest used in the study, and was much higher than the m values used for the other layers in the PTn. The higher the m value, the narrower the distribution of pore sizes for a given matrix sample. Layer ptn22 was previously identified in Figure 3.4.4-2 as having a significant increase in permeability from the initial estimate during the calibration. From this it appears that the samples used in the permeability and van Genuchten estimates may not have been representative of the entire layer across the model domain. This could be a result of the fact that the Tpy can be partially to moderately welded across Yucca Mountain. Perhaps the results of the permeability and van Genuchten studies were biased by samples from these more welded regions.

The preceding plots show that with some exceptions, the most significant changes occurred to the matrix permeability and fracture alpha parameters. The matrix permeability for some layers increased by the same order of magnitude as the infiltration rate. In many cases, a significant change in matrix permeability was correlated with a change in fracture alpha. This correlation was expected before the calibration was performed due to the equivalent capillary pressure conditions which exist in the fractures and matrix due to the steady-state assumption. As the fractures become more saturated at the increased infiltration rates, capillary pressure decline. Permeabilities of the matrix must increase to match the matrix saturation data, and fracture alphas must decrease to maintain equivalent capillary pressures in the fracture and matrix.

Figure 3.4.4-8
Pre- and Post-Calibration Calculated Combined Column Inversion Saturations vs. Measured Data. 0.1 mm/yr case.

Figure 3.4.4-9
Pre- and Post-Calibration Calculated Combined Column Inversion Saturations vs. Measured Data. 5.0 mm/yr case.

Saturation and Capillary Pressure Analysis

Figures 3.4.4-8 and -9 show plots of the calculated saturations for the 0.1 and 5.0 mm/yr uniform infiltration rate inversions with pre- and post-calibration parameters. For an optimal inversion the calibrated data would all fall on the diagonals. However, the plots show that the fit to the data improved markedly through the calibration. The 5.0 mm/yr shows a big improvement, mostly because the uncalibrated model with the initial parameter set provided saturated conditions with large biases as discussed above.

Figure 3.4.4-10
Sensitivity of Matrix Permeability Parameters to Inversion Data at Various Uniform Infiltration Rates.

Saturation and Capillary Pressure Analysis

Figure 3.4.4-11
Sensitivity of Fracture van Genuchten alpha Parameters to Inversion Data at Various Uniform Infiltration Rates.

Figures 3.4.4-10 and -11 show the variability in the overall sensitivities for the matrix permeability and fracture alpha of each layer to the inversion data at each uniform infiltration rate. As discussed above, the overall sensitivity of a parameter is the sum of the absolute sensitivity coefficients scaled by the expected variation of the parameters and the observations. The permeability plot shows that the most sensitive layers are the ptn23, the layers at the boundary of the PTn and TSw (ptn25, tsw31, and tsw32), and the unaltered Prow Pass (pp3pv).

Layer tsw35 is interesting because the matrix permeability is very sensitive at the 0.1 and 1.0 mm/yr infiltration rates, but insensitive at the 0.01 and 5.0 mm/yr rates. A review of Figure 3.4.4-11 showing the fracture alpha sensitivities shows the reverse behavior. For extremely dry or saturated fractures, apparently the fracture alpha must be adjusted to provide equivalent capillary pressures as the measured data are matched. At the two intermediate rates the pressures in the fractures and matrix must be relatively equal so that only the permeability in the matrix has to be adjusted to match the matrix saturation and capillary data.

For the rest of the data in Figure 3.4.4-11, the sensitivity is high at all infiltration rates for layers tcw11, tsw33, and ch3zc. For layer tsw31, however, the frac-

ture alpha sensitivity is high only at the 0.01 mm/yr infiltration rate. This is due to the extremely high matrix permeability sensitivities at the other infiltration rates which dominate the fit to the measured data. Therefore, only when the fractures in this layer are extremely dry is the fracture alpha is sensitive.

Figure 3.4.4-12
Range In Matrix Permeability Parameter Values For 0.1 mm/yr and 5 mm/yr Combined Column Inversions. Ranges are +/- one joint standard deviation.

Figure 3.4.4-12 presents the range in uncertainty for the permeability estimates of the 0.1 mm/yr base case and the 5 mm/yr combined column inversions. The ranges are +/- one joint standard deviation. The results show that even though the parameters of the 0.1 and 5 mm/yr results can be different by orders of magnitude, the estimates generally fall within the ranges for the parameters sets as defined by the joint standard deviation. Therefore, the parameter sets are concluded to be consistent with each other based on the data used in the calibration effort.

Also shown on the figure are the matrix permeability estimates from the Q prior data obtained from the USGS discussed in section 3.2.2.1. The prior data points are generally also within the ranges established by the joint standard deviations, which also indicates that the parameter sets are consistent with the prior information. Also, a comparison with Figure 3.4.4-10 shows that the points with small joint standard deviations are the points with high sensitivities. This means that the more sensitive a parameter is, the lower the resultant uncertainty will be.

3.5 Sensitivity Studies

The calibration efforts using the combined column grid with a range of uniform infiltration rates involved a number of assumptions. The effect of using these assumptions on the calibration results were studied through sensitivity studies. The specific assumptions evaluated, the methodology used, and the results of the analyses are described in the following sections.

3.5.1 Spatially Variable Infiltration Rates

As discussed above, the assumption that uniform net infiltration rates can be used to obtain effective layer parameters is problematic in some aspects. Various hydrologic models have been used to produce spatially variable maps of infiltration at Yucca Mountain. Some factors considered in these models are amount of alluvial cover, contributing watershed area, and slope. The areally averaged estimates from the variable maps range from 1.22 mm/yr (Flint and Flint, 1994) to 4.42 mm/yr (Flint et al., 1996), and tend to be at the upper end of the range of uniform infiltration rates used in this calibration.

Spatially variable infiltration rates to be used in a rate sensitivity study were obtained from the latest infiltration map available from the USGS (Flint et al., 1996). This map will be Q at the end of September, 1996. The rates were obtained by averaging all of the provided infiltration values from Flint et al. (1996) which were within the boundaries of the model gridblock corresponding to a borehole location. However, this averaging had a significant effect on the infiltration associated with a given borehole. The nearest point measurement of infiltration from the map for three of the boreholes was 0.0 mm/yr. This means that there is an assumption of significant spreading and lateral diversion associated with the average gridblock value used in the 1-D inversions. Table 3.5.1-1 provides the infiltration data associated with the spatially variable rate inversion.

Table 3.5.1-1 Spatially Variable Infiltration Rates (mm/yr)		
Borehole	Average Rate	Nearest Point Rate
SD-7	3.6	7.8
SD-9	3.6	10.3
SD-12	2.8	0.0
UZ-14	1.2	0.0
UZ#16	0.6	0.0

Saturation and Capillary Pressure Analysis

Table 3.5.1-2 Residual Standard Deviation(RSD) and Bias Summary for Spatially Variable Infiltration Rates				
Datatype	Run			
	Uncalibrated		Calibrated	
Variable Rates	RSD	Bias	RSD	Bias
Saturation	0.19	-0.14	0.08	-0.03
log (Cap. Pres.)	1.10	50.72	0.66	0.08
SSWRD ¹	448		98	
Infil. Factor				
Saturation	—	—	0.07	-0.01
log (Cap. Pres.)	—	—	0.63	-0.04
SSWRD	—		87	

¹SSWRD= sum of squared weighted residuals

Table 3.5.1-2 shows a summary of the residual standard deviation and bias information provided by the inversion. Although the uncalibrated model has relatively high biases and RSDs, the calibrated parameter set results in a set of RSDs similar to those obtained from the uniform infiltration rate inversions.

A second inversion with the same initial parameter set evaluated the infiltration rates which would provide the best match to the measured borehole data. This was investigated as a factor which would be applied to the variable infiltration rates. The resultant RSDs and biases for the run were among the smallest obtained in the inversions. The factor to be applied to the variable rates estimated from the inversion was 0.025, which results in infiltration rates for the boreholes ranging from 0.02 to 0.09 mm/yr.

The results of these inversions indicate that even though there are uncertainties associated with the variable infiltration rates, it is likely that infiltration does vary spatially at Yucca Mountain. The fact that the range of rates estimated from the infiltration factor analysis had a maximum of 0.09 mm/yr indicates that net average matrix percolation flux at Yucca Mountain may be relatively low. Therefore, as stated previously, higher infiltration rate estimates are probably associated with temporally varying pulses due to extreme storm events. These pulses may proceed through localized structural features with little interaction with the matrix due to fingering and fracture coatings.

3.5.2 Spatially Varying Parameter Distributions

Single column inversions were done to provide an evaluation of the spatial variations in parameter distributions. Since there are numerous parameters estimated in an inversion, there must be as many data points as possible to provide a resultant parameter set with the uncertainties minimized. Therefore, grids for SD-7 and SD-9 were used since those boreholes both have Q saturation and cap-

Saturation and Capillary Pressure Analysis

illary pressure data. The boreholes also include all of the important altered and unaltered hydrogeologic layers down to the bottom of the Prow Pass formation. 1-D columns with node spacings of 2 m were generated for these boreholes. The saturation and capillary pressure data from the USGS were used to generate arithmetically averaged values for the 2 m thick layers. An infiltration rate of 0.1 mm/yr was used for both inversions for easy comparison to the results from the 0.1 mm/yr uniform rate combined grid inversion.

The inversion also tested the effect of using the coarse-grid columns from a 3-D grid for the combined column inversions. For instance, some coarse grid columns from the 3-D UZ model do not resolve all of the vertical heterogeneities known to exist. For instance, the column for borehole SD-9 uses a zeolitic property set in the model layer underlying the TSw basal vitrophyre (chlzc, with associated high saturations), even though the borehole saturation data suggest that a little less than half of the layer is actually vitric with relatively low saturations. However, the layer is too thin to be able to split it into two sub-layers without creating aspect ratio problems in the UZ model.

Figure 3.5.2-1

Borehole SD-7 Calculated Saturations and Capillary Pressures From Fine Grid Column. USGS borehole core sample data from L. Flint.

Saturation and Capillary Pressure Analysis

Figure 3.5.2-2
Borehole SD-9 Calculated Saturations And Capillary Pressures From Fine Grid Column.
USGS borehole core sample data from L. Flint.

Figures 3.5.2-1 and -2 present the simulated and measured saturations and capillary pressure data for the two boreholes. As compared to the results from the coarse grid columns, the simulation results do a better job of matching peaks in the data. For instance, the capillary pressure in the perched water zone in SD-7 was matched by this inversion whereas in the combined column inversion the data from other boreholes prevented this point from being matched. On the other hand, there is the possibility that spurious peaks in the data due to sample handling or measurement errors will be matched by the program and affect the resultant parameter set. Combined column inversions prevent spurious peak matching and smooth out variations in the parameter set to some extent.

The statistical results from the fine grid inversions for SD-7 and SD-7 cannot be directly compared to the other runs because the input data to the inversion was different, making them different inverse problems. Since more data points were generated for use in the inversions from the original USGS core data sets, there was more scatter (due to less averaging) and the RSDs are expected to be larger. The RSDs and biases still provide relative measures of the goodness-of-fits to the borehole data, however.

Saturation and Capillary Pressure Analysis

Table 3.5.2-1 Fine Grid Column Residual Standard Deviation (RSD) and Bias Summary		
	Calibrated Result	
SD-7 Fine-Grid Inversion, 0.1 mm/yr	RSD	Bias
Saturation	0.11	-0.01
Capillary Pressure (log)	0.72	0.08
SD-9 Fine-Grid Inversion, 0.1 mm/yr		
Saturation	0.08	-0.01
Capillary Pressure (log)	0.73	-0.08

The log capillary pressure RSDs and biases were about the same for both inversions indicating that the capillary pressure data are widely scattered but with similar distributions. The biases are almost zero for the measured data sets which means that single column inversions are able to converge to a set of parameters that fit the mean of the data well. The RSD of the saturation data was better for SD-9 than for SD-7 which indicates that there was less scatter in the initial data set for SD-9.

Figure 3.5.2-3

Differences in Matrix Parameter Sets From SD-7 and -9 Fine-Grid Inversions. Baseline is the 0.1 mm/yr inversion parameter set. Log differences used for permeability and alpha parameters. (0.1 case minus fine-grid case).

Figure 3.5.2-4

Differences in Fracture Parameter Sets From SD-7 and -9 Fine-Grid Inversions. Baseline is the 0.1 mm/yr inversion parameter set. Log differences used for permeability and alpha. (0.1 case minus fine-grid case).

Figures 3.5.2-3 and -4 show the differences between the parameter estimates from the 0.1 mm/yr uniform rate inversion and the two fine-grid inversions. The logs of the permeabilities and alpha parameters were used in the difference calculation. A negative number indicates that the log estimate from the 0.1 mm/yr inversion was smaller (smaller absolute permeability) than the result from the fine-grid inversion. There are certain layers which are missing from the fine grid models such as pp22p and ch2vc for SD-9 and ch1zc for SD-7. The differences for these missing layers are shown as zero on the plots.

The results show that the largest differences are in the fracture and matrix permeability estimates, with differences of up to two orders of magnitude from the base case. The largest range is seen in layer pp3vp, the relatively unaltered portion of the Prow Pass, with matrix permeability estimates an order of magnitude smaller and larger than the base case result. This range is probably due to differences in welding and perhaps alteration in the layer between the two boreholes. SD-9 is generally more altered in the CHn than SD-7, and so the reduction in permeability found in this layer is consistent with this alteration pattern. The matrix permeability in layer ch3zc for borehole SD-7 was decreased by more than an order of magnitude over the base case to match the high saturations and low potentials in the perched water zone. The fracture permeability and alpha parameter also had to adjusted to maintain capillary pressure equilibrium.

Even though the coarse-grid column model layer ch1zc for SD-9 combined vitric material with zeolitic material, the differences between the fine- and coarse-grid estimate for ch1zc were small for both the fractures and the matrix parameters. This means that the combination of the two different materials did not have a big effect on the parameter estimates for the model layer.

Figure 3.5.2-5 presents a summary of the conditional standard deviations divided by the resultant parameter estimates. The plot is similar to the normalized data for the 0.1 mm/yr uniform infiltration rate combined column inversion presented previously. However, the normalized matrix permeability uncertainties are significant for more layers. This indicates that the data sets vary more because the data have not been smoothed by layer-averaging, leading to higher uncertainties. The uncertainties associated with the fracture van Genuchten parameters remains high for the same reasons discussed for the 0.1 mm/yr. inversion.

From the fine-grid analysis, it is concluded that single-column inversions can be used to obtain parameter estimates which show spatial variation. However, the process requires numerous data points and so far there are only three boreholes with numerous saturation and water potential data for use in this approach. The inversions also show that in some cases, the assumptions used in the coarse-grid approach combining thin layers with different material properties had no significant effect on the results. The resultant spatial variability demonstrates what effect combining columns with scattered data and perhaps assuming uniform in infiltration rates had on the resultant parameter estimates.

Figure 3.5.2-5
Normalized Conditional Standard Deviation for Model Layer Parameters. SD-9 Fine-Grid Inversion, 0.1 mm/yr. Log values used for permeability and alpha parameters.

**3.5.3
Coupled Permeability and
van Genuchten Alpha
Parameter Study**

The previous sections performed model inversions which allowed all of the matrix and fracture parameters (permeability, and van Genuchten fitting coefficients alpha and m) to vary independently in order to achieve the best fit to the measured data. In reality, the parameters are correlated to some degree. For example, the permeability of a fracture is related to its aperture width. As that width increases, the permeability should increase also. However, as the aperture increases, the van Genuchten alpha parameter related to the inverse of the air entry pressure also increases. Relationships between the two parameters have been proposed by various researchers. Wang (1992) proposed the relationship for the matrix to be:

$$\alpha = f \cdot (k)^{0.5}$$

where: alpha is a van Genuchten fitting coefficient (bars⁻¹)
 f is a factor relating the two parameters
 k is the permeability

For fractures, a relationship can be developed based on the previous equation and using a parallel plate analysis and the cubic law. The relationship is:

$$\alpha = (12 \cdot k)^{0.5} / (2 \cdot \sigma)$$

where: sigma is the surface tension of water.

These relationships were used in an inversion of the combined coarse-grid columns with ITOUGH2. All of the parameters were allowed to vary without regard to their sensitivity to achieve the best fit to the measured data. The results of the inversion and the other sensitivity analyses presented up to this point are shown in Table 3.5.3-1.

Table 3.5.3-1 Sensitivity Study Parameter Sets						
Layer/Parameter		Base Case			Fine-Grid	
Matrix Permeability (m ²)	Prior Data	0.1 mm/yr	Var. Rates	Coupled	SD-7	SD-9
Upper Tpcxxx	1.5E-19	1.6E-19	1.6E-19	4.59E-17	1.6E-19	1.6E-19
Middle Tpcpxxx	5.4E-18	3.4E-17	5.4E-16	2.06E-17	5.4E-16	5.4E-18
Tpcpv3,2	2.2E-17	2.2E-17	2.2E-17	2.76E-17	2.2E-17	2.2E-17
Tpcpv1,Tpbt4	4.0E-13	4.0E-13	4.0E-13	8.46E-15	4.0E-13	4.0E-13
Tpy	3.0E-16	2.4E-13	2.4E-13	9.22E-15	NA	2.4E-13
Tpbt3	5.2E-14	7.6E-15	1.1E-13	2.39E-14	5.2E-14	5.8E-15
Tpp	8.8E-14	8.8E-14	8.8E-14	8.80E-14	NA	7.1E-14
Tpbt2,Tptrv3	4.2E-13	3.1E-13	1.1E-12	4.20E-13	4.2E-13	3.3E-12
Tptrv2,1	1.6E-16	2.5E-15	2.6E-13	1.71E-16	1.6E-16	2.5E-17

Saturation and Capillary Pressure Analysis

Table 3.5.3-1 (cont.)
Sensitivity Study Parameter Sets

Tptrn	1.7E-16	6.8E-15	1.9E-13	6.59E-17	8.8E-16	1.6E-15
Tptrl,Ttpul	2.0E-17	2.1E-18	8.0E-18	2.14E-18	1.3E-18	5.0E-19
Ttpmn	4.0E-18	2.5E-17	1.0E-15	4.28E-19	6.8E-19	3.4E-18
Ttpll	2.3E-17	3.3E-17	4.2E-16	3.80E-18	3.5E-19	1.1E-18
Ttpln	9.6E-17	9.6E-17	7.8E-17	5.23E-19	9.6E-17	9.6E-17
Ttpv3	5.0E-18	2.0E-17	3.2E-16	9.20E-19	5.0E-17	2.0E-15
Ttpv2,1,Tpbt1(z)	5.4E-16	5.4E-16	5.4E-16	4.22E-19	NA	5.4E-16
Ta(z)	4.5E-18	7.1E-19	4.5E-18	1.36E-19	1.1E-19	5.1E-19
Thbt, Prow Un. 4 (z)	8.4E-18	8.4E-18	2.1E-17	9.68E-20	8.4E-18	8.4E-18
Prow Un. 3	3.8E-17	5.2E-16	5.4E-15	7.09E-16	6.3E-15	3.8E-17
Prow Un. 2,1,Tcpbt(z)	1.7E-17	1.7E-17	2.7E-16	1.68E-18	6.8E-18	NA
Ttpv2,1,Tpbt1	1.6E-12	1.6E-12	1.6E-12	3.99E-16	6.9E-14	1.6E-12
Ta	5.5E-14	2.2E-14	5.5E-14	1.06E-16	3.5E-13	NA
Fracture Permeability (m ²)	Prior Data	0.1 mm/yr	Var. Rates	Coupled	SD-7	SD-9
Upper TCw	5.8E-12	6.0E-12	9.1E-12	5.75E-12	2.1E-12	5.8E-12
Middle TCw	5.8E-12	5.8E-12	5.8E-12	5.75E-12	5.8E-12	5.8E-12
Tpcpv3,2	5.8E-12	5.8E-12	5.8E-12	5.75E-12	5.8E-12	5.8E-12
Tptrv2,1	4.0E-12	4.0E-12	4.0E-12	4.00E-12	1.0E-11	6.8E-13
Tptrn	4.0E-12	1.0E-11	4.5E-12	4.00E-11	1.0E-11	3.5E-12
Tptrl,Ttpul	4.0E-12	6.3E-12	7.4E-12	4.00E-12	1.9E-10	2.7E-11
Ttpmn	4.0E-12	4.0E-12	1.6E-12	2.32E-12	4.0E-12	4.0E-12
Ttpll	4.0E-12	4.0E-12	4.0E-12	1.07E-10	5.6E-11	2.1E-11
Ttpln	4.0E-12	4.0E-12	4.0E-12	1.26E-11	4.0E-12	4.0E-12
Ttpv3	1.0E-11	4.0E-12	4.0E-12	4.00E-12	4.0E-12	4.0E-12
Ttpv2,1,Tpbt1(z)	1.0E-13	1.0E-13	1.0E-13	1.00E-13	NA	1.0E-13
Ta(z)	1.0E-13	1.0E-13	1.0E-13	1.00E-13	7.0E-15	3.3E-13
Thbt, Prow Un. 4 (z)	1.0E-13	1.0E-13	1.0E-13	1.00E-11	1.0E-13	1.0E-13
Prow Un. 3	3.0E-14	3.0E-14	3.0E-14	3.00E-14	3.0E-14	3.0E-14
Prow Un. 2,1,Tcpbt(z)	1.0E-13	1.0E-13	1.0E-13	1.00E-13	1.0E-13	NA
Ttpv2,1,Tpbt1	3.0E-14	7.2E-13	7.2E-13	7.23E-13	7.2E-13	7.2E-13
Ta	3.0E-14	7.2E-13	7.2E-13	7.23E-13	7.2E-13	NA
Matrix van Genuchten alpha (1/Pa)	Prior Data	0.1 mm/yr	Var. Rates	Coupled	SD-7	SD-9
Upper TCw	3.4E-06	1.9E-05	1.5E-05	7.8E-07	5.0E-06	3.4E-06
Middle TCw	1.2E-06	1.3E-06	1.7E-06	5.2E-07	2.6E-06	1.1E-06
Tpcpv3,2	2.3E-07	1.4E-06	1.3E-06	6.0E-07	2.3E-07	3.2E-07
Tpcpv1,Tpbt4	3.7E-05	2.2E-05	2.4E-05	1.1E-05	1.4E-05	1.8E-05

Saturation and Capillary Pressure Analysis

Table 3.5.3-1 (cont.) Sensitivity Study Parameter Sets						
Tpy	7.6E-06	1.2E-05	1.6E-05	1.1E-05	NA	3.1E-05
Tpbt3	2.6E-05	3.7E-05	4.5E-05	1.8E-05	2.8E-05	1.2E-04
Tpp	3.4E-05	3.0E-05	3.4E-05	3.4E-05	NA	1.5E-04
Tpbt2,Tptrv3	9.8E-05	1.8E-04	1.4E-04	7.5E-05	3.7E-05	6.4E-04
Tptrv2,1	3.4E-06	2.6E-05	2.4E-05	1.5E-06	5.7E-05	9.8E-05
Tptrn	2.0E-05	1.8E-05	1.7E-05	9.3E-07	5.1E-05	1.2E-05
Tptrl,Tptpul	6.6E-06	6.6E-06	5.7E-06	1.7E-07	4.7E-06	1.1E-05
Tptpmn	6.4E-07	8.0E-07	7.5E-07	7.5E-08	8.1E-07	1.5E-06
Tptpll	2.7E-06	3.5E-06	2.3E-06	2.2E-07	1.1E-06	3.8E-06
Tptpln	4.7E-07	5.6E-07	5.2E-07	8.3E-08	4.6E-07	7.8E-07
Tptpv3	1.0E-07	1.1E-06	8.0E-07	1.1E-07	1.4E-06	4.8E-06
Tptpv2,1,Tpbt1(z)	1.9E-07	1.9E-07	1.9E-07	7.5E-08	NA	1.9E-07
Ta(z)	3.9E-06	5.2E-06	3.9E-06	4.2E-08	6.6E-06	1.9E-06
Thbt, Prow Un. 4 (z)	1.5E-07	1.5E-07	1.5E-07	3.6E-08	1.5E-07	1.5E-07
Prow Un. 3	1.8E-05	2.1E-05	1.9E-05	3.1E-06	8.1E-06	1.1E-05
Prow Un. 2,1,Tcpbt(z)	1.8E-06	1.8E-06	1.3E-06	1.5E-07	5.6E-06	NA
Tptpv2,1,Tpbt1	9.8E-05	9.0E-05	7.6E-05	2.3E-06	6.0E-05	1.9E-05
Ta	9.8E-05	7.2E-05	9.8E-05	1.2E-06	3.1E-05	NA
Frac. van Genuchten alpha (1/Pa)	Prior Data	0.1 mm/yr	Var. Rates	Coupled	SD-7	SD-9
Upper TCw	1.2E-03	1.6E-03	5.2E-04	5.9E-06	9.3E-04	1.2E-03
Middle TCw	1.2E-03	1.2E-03	9.8E-04	5.9E-06	1.2E-03	1.2E-03
Tpcpv3,2	1.2E-03	1.2E-03	1.2E-03	5.9E-06	1.2E-03	1.2E-03
Tptrv2,1	1.2E-03	1.4E-03	1.2E-03	4.9E-06	8.6E-04	2.6E-03
Tptrn	1.2E-03	8.6E-04	9.7E-04	1.6E-05	1.1E-03	1.2E-03
Tptrl,Tptpul	1.2E-03	5.4E-04	2.4E-04	4.9E-06	5.5E-04	7.4E-04
Tptpmn	1.2E-03	1.2E-03	6.9E-04	3.8E-06	1.2E-03	1.2E-03
Tptpll	1.2E-03	1.2E-03	1.1E-03	2.6E-05	4.6E-04	6.2E-04
Tptpln	1.2E-03	1.2E-03	1.2E-03	8.8E-06	1.2E-03	1.2E-03
Tptpv3	1.2E-03	1.2E-03	1.2E-03	4.9E-06	1.2E-03	1.2E-03
Tptpv2,1,Tpbt1(z)	7.3E-04	7.3E-04	7.3E-04	7.8E-07	NA	7.3E-04
Ta(z)	7.3E-04	7.3E-04	3.9E-04	7.8E-07	2.6E-03	2.8E-04
Thbt, Prow Un. 4 (z)	7.3E-04	7.3E-04	7.3E-04	7.8E-06	7.3E-04	7.3E-04
Prow Un. 3	1.2E-03	1.2E-03	1.2E-03	4.3E-07	1.2E-03	1.2E-03
Prow Un. 2,1,Tcpbt(z)	7.3E-04	7.3E-04	7.3E-04	7.8E-07	7.3E-04	NA
Tptpv2,1,Tpbt1	1.2E-03	1.2E-03	1.2E-03	2.1E-06	1.2E-03	1.2E-03
Ta	1.2E-03	1.2E-03	1.2E-03	2.1E-06	1.2E-03	NA

Saturation and Capillary Pressure Analysis

**Table 3.5.3-1 (cont.)
Sensitivity Study Parameter Sets**

Frac. van Genuchten m value	Prior Data	0.1 mm/yr	Var. Rates	Coupled	SD-7	SD-9
Upper TCw	0.20	0.23	0.18	0.20	0.14	0.20
Middle TCw	0.23	0.23	0.22	0.23	0.23	0.23
Tpcpv3,2	0.44	0.44	0.44	0.44	0.44	0.44
Tptrv2,1	0.20	0.20	0.20	0.20	0.20	0.21
Tptrn	0.25	0.25	0.25	0.35	0.31	0.25
Tptrl,Tptpul	0.25	0.27	0.25	0.27	0.34	0.36
Tptpmn	0.32	0.32	0.33	0.32	0.32	0.33
Tptpll	0.23	0.23	0.23	0.36	0.28	0.26
Tptpln	0.42	0.42	0.42	0.44	0.42	0.42
Tptpv3	0.37	0.37	0.37	0.32	0.37	0.37
Tptpv2,1,Tpbt1(z)	0.36	0.36	0.36	0.36	NA	0.36
Ta(z)	0.22	0.23	0.23	0.23	0.24	0.23
Thbt, Prow Un. 4 (z)	0.48	0.48	0.47	0.62	0.48	0.48
Prow Un. 3	0.31	0.31	0.31	0.31	0.31	0.31
Prow Un. 2,1,Tcpbt (z)	0.31	0.31	0.31	0.31	0.31	NA
Tptpv2,1,Tpbt1	0.23	0.23	0.23	0.23	0.23	0.23
Ta	0.23	0.23	0.23	0.23	0.23	NA
Matrix van Genuchten m value	Prior Data	0.1 mm/yr	Var. Rates	Coupled	SD-7	SD-9
Upper TCw	0.20	0.23	0.24	0.18	0.18	0.20
Middle TCw	0.23	0.23	0.23	0.24	0.24	0.23
Tpcpv3,2	0.44	0.46	0.46	0.43	0.43	0.44
Tpcpv1,Tpbt4	0.22	0.22	0.22	0.19	0.22	0.22
Tpy	0.49	0.31	0.31	0.24	NA	0.31
Tpbt3	0.24	0.24	0.24	0.23	0.24	0.24
Tpp	0.30	0.29	0.30	0.22	NA	0.30
Tpbt2,Tptrv3	0.23	0.22	0.24	0.19	0.23	0.23
Tptrv2,1	0.20	0.21	0.21	0.19	0.21	0.21
Tptrn	0.25	0.25	0.25	0.25	0.25	0.26
Tptrl,Tptpul	0.25	0.25	0.25	0.25	0.25	0.25
Tptpmn	0.32	0.32	0.32	0.33	0.32	0.32
Tptpll	0.23	0.22	0.23	0.22	0.22	0.22
Tptpln	0.42	0.41	0.42	0.41	0.41	0.42
Tptpv3	0.37	0.37	0.37	0.36	0.39	0.38
Tptpv2,1,Tpbt1(z)	0.36	0.36	0.36	0.34	NA	0.36
Ta(z)	0.22	0.23	0.23	0.21	0.22	0.22

Saturation and Capillary Pressure Analysis

Table 3.5.3-1 (cont.) Sensitivity Study Parameter Sets						
Thbt, Prow Un. 4 (z)	0.48	0.48	0.48	0.47	0.47	0.48
Prow Un. 3	0.31	0.31	0.32	0.20	0.40	0.31
Prow Un. 2,1,Tcpbt(z)	0.31	0.31	0.31	0.31	0.32	NA
Tptpv2,1,Tpbt1	0.23	0.22	0.22	0.21	0.21	0.19
Ta	0.23	0.22	0.22	0.22	0.28	NA
NA= Layer not present in borehole

Figure 3.5.3-1

Differences in Matrix Parameter Sets From Coupled Parameter And Spatially Variable Infiltration Inversions And Initial Estimate Data Set. Baseline is the 0.1 mm/yr inversion parameter set. Log differences used for permeability and alpha parameters. (0.1 case minus other case).

Figure 3.5.3-2

Differences in fracture parameter sets from coupled parameter and spatially variable infiltration inversions and initial estimate data set. Baseline is the 0.1 mm/yr inversion parameter set. Log differences used for permeability and alpha. (0.1 case minus other case).

Figures 3.5.3-1 and -2 present the differences between the parameter estimates from the 0.1 mm/yr uniform rate inversion and the coupled parameter and spatially variable infiltration inversions. Also included on each plot is the difference between the base case and the initial parameter set. The logs of the permeabilities and alpha parameters were used in the difference calculation. A negative number indicates that the log estimate from the 0.1 mm/yr inversion was smaller (smaller absolute permeability) than the result from the coupled parameter or spatially variable infiltration inversions.

For the variable rate inversion, the matrix permeabilities for many model layers were increased over the base case parameter set. This increase was done to lower saturations in the layers in order to match the measured data. None of the other parameters needed to be changed significantly from the base case result to provide good matches to the measured data.

For the coupled parameter inversion, both the matrix permeability and alpha parameters for many of the layers were decreased significantly over the base case parameters. The resultant parameters can be more than three orders of magnitude smaller than the base case. The fracture properties show an increase in permeability for a few of the layers, but a consistent decrease in fracture

alphas of about two orders of magnitude for all layers. This is a result of having to decrease the alphas to match capillary pressures due to the changed matrix parameters.

The RSD and bias for the saturation data based on the calibrated coupled parameter set are 0.08 and -0.004, respectively. The RSD and bias for the capillary pressure data are 0.62 and -0.06, respectively. These are the best results from any of the combined column inversions. However, many of the significant decreases in matrix properties resulting from the inversion are inconsistent with the extensive matrix property measurements from Flint (1996, in prep.) The change in fracture alphas required to match capillary pressures are also inconsistent with the other inversions at this low infiltration rate in which fracture properties were relatively insensitive and did not vary much. This is shown by the difference between the initial parameter estimates and the base case set shown on the plot. The changes in fracture permeabilities were also inconsistent with the initial estimate set based on the pneumatic data analyses.

The results of the coupled run are inconclusive. On one hand, coupling the parameters makes sense due to the correlation between the permeability and alpha parameters and provided the best fit to the data for any of the combined column runs. On the other hand, the equations relating the parameters are based on some theoretical aspects of matrix and fracture flow with simplifying assumptions. Therefore, the resulting inconsistent parameter set may be due to the use of erroneous relationships. Further research into this topic may be warranted.

3.5.4 Borehole Water Potential Measurements

The combined column inversions described in section 3.4 were developed to achieve the best fit between simulation results and measured saturation and water potential data from borehole core sample measurements. After these inversions were completed, LBNL received a set of preliminary water potential data collected from J. Rousseau of the USGS in July, 1996. Boreholes SD-12, NRG-6, and NRG-7a had sensors which extended into the TSw for a significant portion of the unit. Figure 3.5.4-1 presents a comparison between the layer-averaged core sample data and the in-situ data. The plot shows the significant variability in the data, even in data from the same geologic layer using the same measurement technique.

[illegible]

Comparison of Layer-Average Borehole Core Sample Water Potential Data and In-Situ Measurements. Data from J. Rousseau and L. Flint, USGS.

Table 3.5.4-1 presents a comparison between the results from original combined column inversion at the 0.1 mm/yr uniform infiltration rate described in Section 3.4 and the results obtained with the revised capillary pressure data set. The table shows that the RSDs are smaller with the revised data set, even though the bias of the capillary pressure data has increased slightly due to the elimination of some of the larger capillary pressure data points. Therefore, reducing the scatter in the input data sets provides a somewhat better match to the data.

Table 3.5.4-1 Residual Standard Deviation (RSD) and Bias Summary				
Datatype	Calibrated Data Sets			
	Base Case 0.1 mm/yr.		Revised Cap. Pressures	
	RSD	Bias	RSD	Bias
Saturation	0.09	-0.01	0.08	-0.01
log (Cap. Pres.)	0.66	-0.05	0.61	-0.18

3.5.5 Effects of Sensitivity Limit and Prior Data

The modeling approach used for most of the inversions excluded parameters that were insensitive to the results as discussed in Section 3.3.4. They were excluded from the inversion in an attempt to prevent changes to the prior information contained by the initial estimates unless the matches were improved significantly by the change. However, a test of the effect of using the sensitivity limit to prevent large changes to relatively insensitive parameters was performed with another inversion. This inversion allowed all parameters to be varied without regard to their sensitivities to achieve the best fit possible. The uniform infiltration rate used in the combined column inversion was 0.1 mm/yr.

A second inversion used this same approach; this inversion started with a different initial estimate parameter set in order to investigate the effect of changing the prior information on the inversion results. The revised parameter set was developed prior to receiving the Flint (1996, in prep.) data set. The parameter set was based on Q matrix permeability data from boreholes UZ#16 and SD-9 and individual matrix van Genuchten parameters from boreholes UZN#27 and UZ#16 measured by L. Flint of the USGS. The set had the same initial fracture estimates as were used in all of the other inversions, except that the fracture alphas were decreased by up to an order of magnitude.

Saturation and Capillary Pressure Analysis

Figure 3.5.5-1

Differences in matrix parameter sets from varying all parameters inversion and varying all parameters with different initial parameter estimates inversion. Baseline is the 0.1 mm/yr inversion parameter set. Log differences used for k and alpha.

Figure 3.5.5-2

Differences in Fracture Parameter Sets From Varying All Parameters Inversion And Varying All Parameters With Different Initial Parameter Estimates Inversion. Baseline is the 0.1 mm/yr inversion parameter set. Log differences used for k and alpha.

Figures 3.5.5-1 and -2 were created to show the differences between the resultant parameter sets for the inversions varying all parameters and using revised initial estimates. Also included for comparison is the difference between the initial parameter set and the base case results. The differences were obtained in the same manner as the plots discussed in the preceding sections. Figure 3.5.5-1 shows the results for the matrix parameters, and Figure 3.5.5-2 shows the results for the fracture parameters obtained from the inversions.

The inversion which showed the most variation from the matrix parameters of the base case was the one in which the parameters were allowed to vary without regard to their sensitivities and with a revised initial estimate set. Some matrix permeabilities and alpha parameters were different from the base case by as much as 2 orders of magnitude. Fracture alpha parameters were also consistently decreased for all of the model layers, consistent with changes to the initial data set.

The inversion which had the same original estimate data set as the preceding inversions but allowed the parameters to be varied without regard to their sensitivities also showed differences from the base case. However, the differences were smaller than in the inversion where the initial parameter set was different.

From these inversions, it is concluded that the effect of allowing all parameters to be varied without regard to their sensitivities was significant, but altering the initial estimate data set had more effect. This highlights the importance of developing an initial parameter set with uncertainties minimized based on measured data. This is especially important in the case of the fracture parameter set which is based on limited non-Q data. The parameter sets obtained from these runs do not preserve the information obtained from extensive matrix measurements and can lead to inconsistently variable properties between adjacent layers with similar characteristics.

3.5.6 Additional Work

The parameter sets from some of these inversions were used in simulations done with the full 3-D model. Ahlers et al. (1995) previously showed that using the parameters from the 1-D inversions in the 3-D grid did not significantly affect the calculated saturation and capillary pressure profiles. The results of the runs using the parameter sets obtained through these inversions are described by Wu et al. in Chapter 6 of this report.

3.6 Conclusion

3.6.1 Q Status of Study

The work performed in this study is documented in Yucca Mountain Project Scientific Notebook YMP-LBNL-GSB-1. The Q status of the data used in the analyses are as follows:

Saturation and Capillary Pressure Analysis

- The borehole data set used in the inversions is presently Q, with the exception of the lower portions of boreholes SD-7 and SD-12.
- The in-situ borehole potentials used in a sensitivity analysis will be submitted to the Technical Database (TDB) by the end of fiscal year 1996.
- Q borehole logs were used to develop the 1-D columns used in the inversions. SD-7 and -12 logs will be Q by September, 1996.
- The TOUGH2 code used to calculate the saturations and capillary pressures in the 1-D grids is Q.
- The ITOUGH2 code used in the inversions and which provided the standard deviations and sensitivities used in the uncertainty and sensitivity analyses is Q.
- The initial matrix property estimates provided by L Flint will be submitted to the TDB by the end of FY96, and will be Q.
- The spatially variable infiltration rate map will be Q by the end of FY96.
- The fracture van Genuchten parameters provided by the TSPA-93 reference are not Q parameters. The fracture permeability estimates provided by Ahlers et al. (1996) will be Q data when the pneumatic data sets the analysis is based on is submitted to the TDB.

Therefore, when the final Q data sets are submitted to the TDB and the ITOUGH2 code has been given Q status, the only non-Q data used in the study will be the fracture van Genuchten parameters.

In FY97, LBNL will use fracture frequency data from the ESF and from Q boreholes to develop a new fracture van Genuchten parameter set following the methodology outlined in TSPA-93. The inversions will then be redone with this revised parameter set after verifying that all of the above presently non-Q data have become Q. The results of the inversions will then become Q and will be provided to Yucca Mountain Project participants.

3.6.2 Conclusions

Based on the evaluations done during this calibration, the following conclusions are reached:

1. The ECM formulation provides the same simulated profiles as a dual-k formulation under steady-state conditions. Under this condition, the matrix and fracture capillary pressures are equivalent.

2. Grids consisting of layers which explicitly represent the major geological formations and altered zones in the UZ provide sufficient resolution to match the borehole data.
3. The fit between the observed and calculated saturation and capillary pressure profiles could be improved during the calibration process by updating some of the model parameters. Therefore, the conceptual model of steady-state conditions in the UZ based on the matrix core sample data is validated.
4. The 0.1 mm/yr inversion had the smallest residual standard deviations (RSD) for the uncalibrated parameter set. The best uniform rate calibrated fit was achieved for the rate of 0.01 mm/yr. The fact that the best fits to the data with the initial parameter set and the calibrated parameters occurred at the 0.1 and 0.01 mm/yr rates, respectively, may suggest that the net percolation flux through the matrix based on matrix properties is relatively low. However, the differences among the RSDs and biases of the calibrated parameter sets are too small to confirm this. Also, the fact that the calibrations are slightly better for the decreased infiltration rates does not preclude higher overall rates occurring as transient pulsed flow through localized structural features. This flow may be responsible for transporting environmental isotopes into the mountain.
5. The calibrated RSDs and biases increased slightly at the higher rates of 1.0 and 5.0 mm/yr. This may be an indication that the steady-state conditions assumed for the higher infiltration rates may be unrealistic and that the increases are due to the fact that higher infiltration rates are related to the transient pulsed flows discussed in Conclusion 4. If the "actual" average annual rate is similar to one of the higher rates used in this study, it is possible the uniform rate assumption for all boreholes at these higher fluxes is unrealistic, especially since a number of spatially variable infiltration maps have been developed for the project.
6. The spatially variable rate inversion with significant infiltration rates provided fits to the measured data which were at least as good as the uniform rate inversions. This indicates that the conceptual model of spatial variability of infiltration at Yucca Mountain is compatible with the numerical model. The factor of 0.025 estimated from the spatially variable rate inversion to be applied to the spatially variable rate map is another indication that the net percolation flux through the matrix may be relatively small. Again, the higher estimate rates recently estimated by project staff may be related to transient flows through localized structural features rather than average annual rates.
7. The standard deviations for many of the resultant parameters are very large, which indicates that the information contained in the saturation and

capillary pressure data available at this time are insufficient to determine model parameter sets which are unique and highly constrained. Additional data would provide estimates which are more tightly constrained. However, the calibrated model is able to better reproduce the system behavior on a large scale.

8. As the infiltration rate increases, the two parameters that are most sensitive to providing good matches to the data are the matrix permeability and the fracture van Genuchten alpha parameter. The matrix permeability increases on the order of the infiltration rate increase for many model layers. As the matrix permeability is decreased to match measured saturations and fractures saturations increase, the fracture alpha must be decreased to maintain capillary pressure equilibrium.
9. The van Genuchten m values do not vary much and are not sensitive. Thus, they do not contribute much towards improving the fit. Fracture permeability and matrix van Genuchten alpha values show limited sensitivities, with some exceptions. The parameters which show the highest sensitivity during the 0.1 mm/yr inversion are the matrix permeability and the fracture alpha.
10. Better matches to the data can be obtained by allowing the parameters to vary without regard to sensitivity. However, the resultant parameter set does not preserve the information obtained from extensive matrix measurements and can lead to inconsistently variable properties between adjacent layers with similar characteristics.
11. From the results of the fine-grid analysis, it is concluded that single-column inversions can be used to obtain parameter estimates which vary spatially. However, the process requires numerous data points and so far there are only three boreholes with numerous saturation and water potential data for use in this approach. Due to significant scatter in the core sample data, matching peaks in the data may provide parameter estimates with apparent variations which are related more to sampling effects rather than in-situ conditions. The uncertainties in the resultant data sets are larger than in the combined column approach because the data are not smoothed by averaging across coarse model layers.
12. The fine-grid inversions also show that in some cases, the assumptions used in the coarse-grid approach combining of thin layers with different material properties had no significant effect on the results. The resultant spatial variability in the fine-grid inversion results also indicates that applying uniform infiltration rates to the combined column inversions may have had some effect on the resultant parameter estimates.
13. A comparison between the inversion at the 0.1 mm/yr uniform infiltration rate and the results obtained with the revised capillary pressure data set

show that the RSDs are better with the revised data set, even though the bias of the capillary pressure data increased slightly. Therefore, reducing the scatter in the input data sets provides a better match to the data.

14. The results of the coupled parameter inversion are inconclusive. On one hand, coupling the parameters makes sense due to the correlation between the permeability and alpha parameters and provided the best fit to the data for any of the combined column runs. On the other hand, the matrix permeability estimates from the inversion are significantly different than the values provided from extensive matrix measurements. This leads to less confidence in the results. However, the equations relating the parameters are based on some theoretical aspects of matrix and fracture flow with simplifying assumptions. Therefore, the results may be due to the use of equations which do not describe the correlations sufficiently. Further research into this topic may be warranted.
15. The effect of using a sensitivity cutoff limit is less than the effect of altering the initial estimate data set. The parameter sets obtained from these runs do not preserve the information obtained from extensive matrix measurements and lead to inconsistently variable properties between adjacent layers with similar characteristics.
16. The best estimate sets from this study are concluded to be: 1) The results from the 0.1 mm/yr uniform infiltration rate for uniform rate studies due to the good uncalibrated and calibrated fits; and 2) The results from the spatially variable map inversion due to the good calibrated fit if higher or spatially variable infiltration rates are used. However, the fits with the various parameter sets are all reasonable based on the statistical results.

3.6.3

Future Work

Future work to refine the calibration efforts of this study include developing additional refined grids to be able to characterize the spatial variability of the hydrogeologic parameters at all boreholes with available data. As part of this effort, the saturations estimated from geophysical log data currently being developed by M&O staff will be used. Other spatially variable infiltration rate patterns will be included in the calibration studies as they become available. Additional work to develop a Q fracture property set to use in the calibration as described in the Q status section of this report will also be done.

3.7 References

- Ahlers C.F., et al, Summary of model calibration and sensitivity studies using the LBNL/USGS three-dimensional unsaturated zone site-scale model. Lawrence Berkeley National Laboratory, 1995.
ACCN: MOL.19960208.0091-0097
DTN: LB092995312293.001
- Ahlers C.F., C. Shan, C. Haukwa, A.J.B. Cohen, G.S. Bodvarsson, Calibration and prediction of pneumatic response at Yucca Mountain, Nevada using the LBNL/USGS three-dimensional, site-scale model of the unsaturated zone, Yucca Mountain Project Milestone OB12M, 1996.
- Anna L., Preliminary Three-Dimensional Discrete Fracture Model, Tiva Canyon Tuff, Yucca Mountain Area, Nye County, Nevada, Water Resources Investigations Report, 1996. (In Prep.)
DTN: GS960408312281.001 (Q)
- CRWMS M&O, Total System Performance Assessment - 1995: An Evaluation of the Potential Yucca Mountain Repository, Document B00000000-01717-2200-00136, Rev. 01, 1995.
- Fabryka-Martin J.T., P.R. Dixon, S. Levy, B. Liu, H.J. Turin, A.V. Wolfsberg, Summary Report of Chlorine-36 Studies: Systematic sampling for Chlorine-36 in the Exploratory Studies Facility. LANL Level 4 Milestone Report 3783AD, March 29, 1996.
- Finsterle S., ITOUGH2 User's Guide Version 2.2, Report LBNL-34581, Lawrence Berkeley National Laboratory, Berkeley, CA, 1993.
ACCN: MOL.19941026.0075
- Flint A.L., L.E. Flint, Spatial distribution of potential near surface moisture flux at Yucca Mountain, in Proceedings of the Fifth International High Level Radioactive Waste Management Conference, Las Vegas, NV, May 22-26, 1994, pp. 2352-2358, American Nuclear Society, La Grange Park, Ill., 1994.
- Flint L.E., A.L. Flint, Preliminary Permeability and Water-Retention Data for Non-welded and Bedded Tuff Samples, Yucca Mountain Area, Nye County, Nevada, USGS OFR-90-569, YMP DTN GS920108312231.006, 1990.
ACCN: NNA.19890630.0005
DTN: GS92010831231.006 (Non-Q)
- Flint L.E., Matrix properties of hydrogeologic units at Yucca Mountain, Nevada, USGS report, 1996 (In Prep.)
DTN: GS950308312231.002 (Q)

Saturation and Capillary Pressure Analysis

- Flint L.E., A.L. Flint, The influence of long term climate change on net infiltration at Yucca Mountain, Nevada, Proceedings of the Fourth International High Level Radioactive Waste Management Conference, Las Vegas, NV, April 26-30, 1993, pp. 152-159, American Nuclear Society, La Grange Park, Ill., 1993.
ACCN: NNA.19930615.0054
- Ho C.K., S.J. Altman, B.W. Arnold, Alternative Conceptual Models and Codes for Unsaturated Flow in Fractured Tuff: Preliminary Assessments for GWTT-95, Yucca Mountain Site Characterization Project Report, SAND95-1456, September 1995.
- Klavetter E.A., R.R. Peters, An Evaluation of the Use of Mercury Porosimetry in Calculating Hydrologic Properties of Tuffs From Yucca Mountain, Nevada, SAND86-0286, 1987.
ACCN: NNA.19890327.0056
- Klavetter E.A., R.R. Peters, Estimation of hydrologic properties of an unsaturated fractured rock mass, SAND83-2593, Sandia National Laboratories, 1986.
- Kume J., D.P. Hammermeister, Geohydrologic data for well USW H-6, Yucca Mountain Area, Nye Country, Nevada, us Geological Survey Open-File Report 88-465, p.37, 1990.
- Kume J., D.P. Hammermeister, Geohydrologic data from drill-bit cuttings and rotary cores from test hole USW UZ-13, Yucca Mountain Area, Nye County, Nevada, Open-File Report 90-362, U.S. Geological Survey, Denver, CO, 1991.
ACCN: NNA.19901015.0196
- Lecain G.D., J.N. Walker, Results of Air-Permeability Testing in a Vertical Borehole at Yucca Mountain, Nevada, Proceedings of the Fifth Annual International Conference High Level Radioactive Waste Management, Las Vegas, Nevada, May 22-26, 1994.
ACCN: NNA.19940829.0015
- Loskot C.L., Geohydrologic data from test hole USW UZ-6s, Yucca Mountain, Nye County, Nevada, Open-File Report 93-60, U.S. Geological Survey, Denver, CO, 1993.
ACCN: MOL.19941006.0051
DTN: GS921208312211.013 (Non-Q)
- Loskot C.L., D.P. Hammermeister, Geohydrologic data from test holes UE-25 UZ #4 and UE-25 UZ #5, Yucca Mountain Area, Nye County, Nevada, Open-File Report 90-369, U.S. Geological Survey, Denver, CO, 1992.
ACCN: NNA.19880829.0094
DTN: GS921008312211.008 (Non-Q)

Saturation and Capillary Pressure Analysis

- Mishra S., Y. Xiang, B. Dunlap, Analysis of steady-state infiltration into Yucca Mountain using 1-D and 2-D models: preliminary results, TRW Environmental Safety System Inc., Document No. B00000000-01717-0200-00123, Las Vegas, NV, September 1994.
ACCN: MOL.19950313.0048
- Persoff P., K. Pruess, Two-Phase Flow Experiments in Natural Rock Fractures from Yucca Mountain, LBL-37716, September 1995.
DTN: LB092195831129.001 (Q)
- Peters R.R.; E.A. Klavetter, I.J. Hall, S.C. Blair, P.R. Heller, G.W. Gee, Fracture and Matrix Hydrologic Characteristics of Tuffaceous Materials From Yucca Mountain, Nye County, Nevada, SAND84-1471, (SNSAND84147100.000), 1984.
ACCN: NNA.19900810.0674
- Pruess K., TOUGH User's Guide, Nuclear Regulatory Commission Report NUREG/CR-4645, NRC, Washington, DC, 1987. Also published as Report LBNL-20700, Lawrence Berkeley National Laboratory, Berkeley, CA, August 1987.
ACCN: NNA.19890315.0010
- Pruess K., TOUGH2- A general purpose numerical simulator for multiphase fluid and heat flow, Lawrence Berkeley National Laboratory Report LBL-29400, Lawrence Berkeley National Laboratory, Berkeley, CA, May, 1991.
ACCN: NNA.1940202.0088
- Rousseau, J.P., E.M. Kwicklis, C. Gillies, ed.s, Hydrogeology of the Unsaturated Zone, North Ramp Area of the Exploratory Studies Facility, Yucca Mountain, Nevada, USGS WRI-96xxxx, 1996.
- Schenker AR, D.C. Guerin, T.H. Robey, C.A. Rautman, R.W. Barnard, Stochastic Hydrogeologic Units and Hydrogeologic Properties Development for Total-System Performance Assessments, Yucca Mountain Site Characterization Project Report, SAND94-0244, September, 1995.
- Sweetkind D.S, E.R. Verbeek, J.K. Geslin, T.C. Moyer, Fracture Character of the Paintbrush Tuff Nonwelded Hydrologic Unit, Yucca Mountain, Nevada, USGS Administrative Report, 1996.
DTN: GS950808314222.006 (Q)
- Thamir Falah, E.M. Kwicklis, S. Anderton, Laboratory Study of Water Infiltration into a Block of Welded Tuff, In Proceedings of the Fourth Annual International Conference on High Level Radioactive Waste Management, Sponsored by the American Nuclear Society and American Society of Civil Engineers, Las Vegas, Nevada, pp.2071-2080, April 26-30, 1993.
ACCN: NNA.19940120.0066
DTN: GS921208312242.002 (Non-Q)

Thoma S.G., D.P. Gallegos, D.M. Smith, Impact of Fracture Coatings on Fracture/Matrix Flow Interactions in Unsaturated, Porous Media., Water Resources Research, Vol. 28, No. 5, pp. 1357-1367, May, 1992.

Wang J.S.Y., Variations of hydrological parameters of tuff and soil, Proceedings of the Third International Conference on High Level Radioactive Waste Management, Las Vegas, NV, pp.77-731, American Nuclear Society, La Grange Park, Ill., 1992.
ACCN: MOL.19950223.0067

Wang J.S.Y., T.N. Narasimhan, Hydrologic mechanisms governing fluid flow in a partially saturated, fractured, porous medium, Water Resources Research, V. 21, No. 12, pp. 1861-1874, 1985.
ACCN: NNA.19891109.0050
DTN: SNL15041284001.001 (Non-Q)

Weeks E.P., Effect of topography on gas flow in unsaturated fractured rock: concepts and observations, flow and transport through unsaturated fractured rock, (D.D. Evans and T.J. Nicholson, Eds.), Geophysical Monograph 42, American Geophysical Union, Washington, D.C., pp.165-170, 1987.
ACCN: HQS.19880517.3214

Wilson M.L., J.H. Gauthier, R.W. Barnard, G.E. Barr, E.D. Dockery, R.R. Eaton, D.C. Guerin, N. Lu, M.J. Martinez, R. Nilson, C.A. Rautman, T.H. Robey, B. Ross, E.E. Ryder, A.R. Schenker, S.A. Shannon, L.H. Skinner, W.G. Halsey, J.D. Gansemer, L.C. Lewis, A.D. Lamot, I.R. Triay, A. Meijer, D.E. Morris, Yucca Mountain Site Characterization Project, Total-System Performance Assessment for Yucca Mountain - SNL Second Iteration (TSPA-1993), SAND93-2675, Executive Summary, 1993.
ACCN: NNA.19940112.0123

Wittwer C., G. Chen, G.S. Bodvarsson, M. Chornack, A. Flint, L. Flint, E. Kwicklis, R. Spengler, Preliminary development of the LBL/USGS three-dimensional site-scale model of Yucca Mountain, Nevada, Report LBL-37356, UC-814, Lawrence Berkeley National Laboratory, Berkeley, CA, 1995.

**COMPUTER MODELS AND THEIR
DEVELOPMENT FOR THE
UNSATURATED ZONE MODEL
AT YUCCA MOUNTAIN**

Y.S. Wu, S. Finsterle and K. Pruess

August 1996

4.1 Introduction

Quantitative evaluation of moisture, gas and heat flow, and their effects on the performance of the potential high-level nuclear waste repository at Yucca Mountain is essential for conducting site characterization studies and designing the repository and the engineered barrier system. Numerical modeling has played a crucial role in understanding the impact of the unsaturated-zone fluid movement, and the effect of hydrogeologic and thermal conditions on various aspects of the overall waste disposal system. While laboratory and field experiments are limited in space and time, numerical modeling provides a means to study physical processes on the temporal and spatial scales that are relevant for the understanding of a nuclear waste in a geologic formation. Performance assessment models based on numerical simulation of water, gas and heat flow can include all the important physical and chemical processes that affect the behavior of the repository and the host rock.

Numerical modeling approaches for simulating fluid flow and thermal loading processes are generally based on methodologies developed for geothermal and petroleum reservoir simulation. They involve coupled multiphase fluid and heat flow formulations based on finite difference or finite element schemes. The methodology developed in these industries has been enhanced to deal with the hydrologic and thermal conditions encountered in the vicinity of high-level nuclear waste packages. Available numerical simulators for variably saturated nonisothermal flow generally employ mathematical and numerical methods similar to those used in the oil industry. Since the oil and geothermal industries have different priorities than organizations dealing with nuclear waste repository assessment, the codes must account for a number of additional processes such as the slow movement of fluids over very long time periods. The improvement of the modeling capabilities for simulating field-scale problems has been subject to continuous research efforts, and considerable progress in this area has been made over the past two decades.

A number of numerical computer models for evaluating the unsaturated-zone hydrologic conditions at Yucca Mountain have been developed (Wittwer et al., 1995; Ahlers et al., 1995a,b). Modeling coupled processes in large-scale, three-dimensional, fractured systems is conceptually difficult and computationally demanding. As discussed in Chapter 6 (Doughty et al., 1996), the effective-continuum method (ECM) is a good approximation to explicit modeling of fracture-matrix interaction whenever steady-state or near steady-state conditions prevail.

The TOUGH2 code (Pruess, 1991) has been used extensively in modeling thermohydrologic processes at Yucca Mountain because of its flexibility and robustness in handling multi-dimensional, multiphase, and multi-component fluid flow and heat transfer in porous and fractured rocks.

Throughout the development of the MULKOM/TOUGH codes, a comprehensive verification and validation study has been conducted (Pruess, 1991; and Moridis and Pruess, 1992). The correctness, the validity, and the capability of the TOUGH2 family of codes have been verified by comparing the simulation results against analytical solutions, other numerical codes, laboratory experiments, and field observations. The TOUGH2 code has proven itself to be a reliable, accurate, and efficient predictive tool for simulating non-isothermal flow and transport phenomena in variably saturated rocks.

Inverse modeling capabilities for TOUGH2 were developed by Finsterle (1993). The main purpose of ITOUGH2 (Inverse TOUGH2) is to estimate hydrogeologic model parameters for the TOUGH2 code by automatically calibrating the model against observed laboratory and field data. In addition, ITOUGH2 provides a detailed residual and error analysis of the estimated parameter set, and allows examining the uncertainty of model predictions by either first-order-second-moment error propagation analysis or Monte Carlo simulations. Applications of ITOUGH2 for model calibration and sensitivity studies are discussed in Chapter 3 (Bandurraga et al., 1996) and Ahlers et al., 1995a, 1995b, 1996).

A comprehensive code verification and benchmarking study of TOUGH2 has been completed at LBNL, and TOUGH2 (Standard Version 1.11) has been qualified for characterization studies at Yucca Mountain (Pruess et al., 1996). ITOUGH2 software qualification is described in Wu et al., 1996.

In this work we report the recent developments in the computer programs used for studying flow and transport at Yucca Mountain. The main TOUGH2 module has been continuously updated, enhanced, and modified to account for additional processes. Furthermore, ITOUGH2 has been used for model calibration and parameter estimation. In this report, we will give a brief summary of the computer codes used and the newly-implemented options, and discuss some modeling issues. Also, it should be mentioned that there are neither Q nor non-Q used in this chapter, since this chapter deals with the computer models and development.

4.2 TOUGH2 Code

The TOUGH2 code was developed at the Lawrence Berkeley National Laboratory for simulating multi-dimensional coupled fluid and heat flows of multiphase, multi-component fluid mixtures in porous and fractured media

(Pruess, 1991). TOUGH2 belongs to the MULKOM family of codes (Pruess, 1988), and is an enhanced version of the TOUGH simulator (Pruess, 1987).

TOUGH2's predecessor is the code MULKOM ("MULTi-KOMponent"; Pruess, 1983b). MULKOM featured a modular architecture, in which a central module for flow and transport could be interfaced with several different fluid property modules to model systems with different fluid mixtures. The coding of MULKOM evolved into a collection of program modules for specialized applications. Nuclear-waste oriented applications spurred an effort to finalize and document a version of MULKOM for non-isothermal two-phase flows of water and air, which became TOUGH (Transport Of Unsaturated Groundwater and Heat) (Pruess, 1987), and TOUGH2 (Pruess, 1991).

4.2.1 Mathematical Formulation of Mass and Energy Balance

The TOUGH2 simulator takes into account non-isothermal flow of the two components water and air in two phases (liquid and gas), as well as heat flow through porous and fractured geological media. Fluid flow in both liquid and gaseous phases occurs under pressure, viscous, and gravity forces according to Darcy's law, with interference between the phases represented by means of relative permeability functions. Mass- and energy-balance equations are written in integral form for an arbitrary flow domain. In addition, TOUGH2 considers binary diffusion in the gas phase, as well as a simplified description of Knudsen diffusion by means of a Klinkenberg factor for permeability (Knudsen, 1909; Klinkenberg, 1941; Hadley, 1982). Capillary pressure, vapor adsorption, and vapor pressure lowering effects are taken into account.

The transport equations are complemented with constitutive relationships, which express all parameters as functions of a set of thermodynamic variables. All thermophysical properties of liquid water and vapor are obtained within experimental accuracy from steam tables (International Formulation Committee, 1967). Air is treated as an ideal gas, and additivity of partial pressures is assumed for air/vapor mixtures. The viscosity of air/vapor mixtures is computed from a formulation given by Hirschfelder et al. (1954), using steam table values for vapor viscosity. Air solubility in liquid water is represented by Henry's law. The temperature dependence of Henry's constant is neglected because of the generally low air solubility in water.

Heat transport occurs by means of (a) conduction, with thermal conductivity dependent on water saturation, (b) convection, and (c) binary diffusion which includes both sensible and latent heat. The description of thermodynamic conditions is based on a local equilibrium assumption of all phases.

The governing equations and their numerical implementation used in TOUGH2 are applicable to one-, two-, or three-dimensional, heterogeneous and anisotropic porous or fractured media. TOUGH2 does not perform deformation analysis of the host medium and its effects on the multiphase flow behav-

ior, but it allows for porosity changes in response to changes in pore pressure (compressibility) and temperature (expansivity).

The basic mass- and energy-balance equations solved by TOUGH2 can all be written in the following general form (Pruess, 1991):

$$\frac{d}{dt} \int_{V_n} M^{(\kappa)} dV = \int_{\Gamma_n} \mathbf{F}^{(\kappa)} \cdot \mathbf{n} d\Gamma + \int_{V_n} q^{(\kappa)} dV \quad (4.2.1.1)$$

The integration here is over an arbitrary subdomain V_n of the flow system under study, which is bounded by the closed surface Γ_n . The quantity M appearing in the accumulation term denotes mass or energy per unit volume, with $\kappa = 1, \dots, NK$ labeling the mass components, and $\kappa = NK + 1$ for the heat "component". NK is the total number of chemical components.

The general form of the mass accumulation term is

$$M^{(\kappa)} = \phi \sum_{\beta=1}^{NPH} S_{\beta} \rho_{\beta} X_{\beta}^{(\kappa)} \quad (4.2.1.2)$$

The total mass of component κ is obtained by summing over all fluid phases $\beta = 1, \dots, NPH$. NPH is the total number of phases considered. ϕ is the porosity, S_{β} is the saturation (volume fraction of the pore space) of phase β , ρ_{β} is the density of phase β , and $X_{\beta}^{(\kappa)}$ is the mass fraction of component κ present in phase β . The heat accumulation term in a multi-phase system is

$$M^{(NK+1)} = \phi \sum_{\beta=1}^{NPH} S_{\beta} \rho_{\beta} u_{\beta} + (1 - \phi) \rho_R C_R T \quad (4.2.1.3)$$

where u_{β} denotes internal energy of fluid phase β .

The mass flux term is the sum over the NPH phases

$$\mathbf{F}^{(\kappa)} = \sum_{\beta=1}^{NPH} X_{\beta}^{(\kappa)} \mathbf{F}_{\beta} \quad (4.2.1.4)$$

for $\kappa = 1, \dots, NK$. Individual phase fluxes are given by a multi-phase version of Darcy's law:

$$F_{\beta} = -k \frac{k_{r\beta}}{\mu_{\beta}} \rho_{\beta} (\nabla P_{\beta} - \rho_{\beta} \mathbf{g}) \quad (4.2.1.5)$$

Here k is the absolute permeability, $k_{r\beta}$ is the relative permeability of phase β , μ_{β} is viscosity. The term

$$P_{\beta} = P + P_{c,\beta} \quad (4.2.1.6)$$

is the pressure of phase β , which is the sum of the pressure P of a reference phase, and the capillary pressure $P_{c,\beta}$ of phase β relative to the reference phase. $\mathbf{g}$ denotes the vector of gravitational acceleration. The gas phase permeability is described by the Klinkenberg relationship $k = k_{\infty}(1 + b/P)$, where k_{∞} is the absolute permeability at high pressures, and b is the Klinkenberg gas slip factor (Klinkenberg, 1941).

In addition to Darcy flow, TOUGH2 accounts for binary diffusion in the gas phase for fluids with two gaseous (or volatile) components according to the relationship

$$f_{\beta=\text{gas}}^{(\kappa)} = -\phi S_g \tau D_{\kappa\kappa'} \rho_g \nabla X_g^{(\kappa)} \quad (4.2.1.7)$$

where $D_{\kappa\kappa'}$ is the coefficient of binary diffusion, depending on the nature of the gaseous components as well as on pressure and temperature, and τ is a tortuosity factor. The flux-term (4.2.1.7) is simply added to that the mass flux $F^{(\kappa)}$ in (4.2.1.4).

Neglecting dispersion, the heat flux contains conductive and convective components

$$\mathbf{F}^{(NK+1)} = -K \nabla T + \sum_{\beta} h_{\beta} F_{\beta} \quad (4.2.1.8)$$

where K is the thermal conductivity of the medium, T is temperature, and $h_{\beta} = u_{\beta} + P/\rho_{\beta}$ is the specific enthalpy of phase β .

4.2.2
Numerical Scheme - IFD

The continuum equations (4.2.1.1) are discretized in space using the "integral finite difference" (IFD) method (Edwards, 1972; Narasimhan and Witherspoon, 1976). Introducing appropriate volume averages, we obtain

$$\int_{V_n} M dV = V_n M_n \quad (4.2.2.1)$$

where M is a volume-normalized extensive quantity, and M_n is the average value of M over V_n . Surface integrals are approximated as a discrete sum of averages over the surface segments A_{nm} :

$$\int_{\Gamma_n} \mathbf{F}^K \cdot \mathbf{n} d\Gamma = \sum_m A_{nm} F_{nm} \quad (4.2.2.2)$$

where F_{nm} is the average value of the (inward) normal component of $\mathbf{F}$ over the surface segment A_{nm} between the adjacent volume elements V_n and V_m . The discretization approach used in the integral finite difference method and the definition of the geometric parameters are illustrated in Fig. 4.2.1.

Figure 4.2.1
Space discretization and geometry data in the integral finite difference method.

The discretized flux is expressed in terms of averages of parameters for elements V_n and V_m . From the basic Darcy flux term, Eq. (4.2.1.5), we obtain

$$F_{\beta,nm} = -k_{nm} \left[\frac{k_{r\beta} \rho_{\beta}}{\mu_{\beta}} \right]_{nm} \left[\frac{P_{\beta,n} - P_{\beta,m}}{D_{nm}} - \rho_{\beta,nm} g_{nm} \right] \quad (4.2.2.3)$$

where the subscripts (nm) denote a suitable averaging at the interface between grid blocks n and m (interpolation, harmonic weighting, upstream weighting). D_{nm} is the distance between the nodal points n and m, and g_{nm} is the component of gravitational acceleration in the direction from m to n.

The discretized form of the binary diffusive flux in the gas phase is

$$J_{g,nm}^{\kappa} = - \left(\phi S_g \tau_g \right)_{nm} \left(D_g^{\kappa} \right)_{nm} \rho_{g,nm} \frac{X_{g,n}^{\kappa} - X_{g,m}^{\kappa}}{D_{nm}} \quad (4.2.2.4)$$

For the group $(\phi S \tau)$ geometric weighting is used at the interface, while D and ρ are averaged between grid blocks n and m.

Substituting Eqs. (4.2.2.1) and (4.2.2.2) into the governing Eq. (4.2.1.1), a set of first-order ordinary differential equations in time is obtained.

$$\frac{dM_n^{\kappa}}{dt} = \frac{1}{V_n} \sum_m A_{nm} F_{nm}^{\kappa} + q_n^{\kappa} \quad (4.2.2.5)$$

Time is discretized using a first order finite difference approximation, and the flux and sink and source terms on the right hand side of Eq. (4.2.2.5) are evaluated at the new time level, $t^{k+1} = t^k + \Delta t$, to obtain the numerical stability needed for an efficient calculation of multiphase flow. This treatment of the flux terms is known as "fully implicit," because the fluxes are expressed in terms of the unknown thermodynamic parameters at the new time level t^{k+1} , and these unknowns are defined implicitly in the resulting equations (Peaceman, 1977). The time discretization results in the following set of coupled non-linear, algebraic equations

$$- \sum_i \frac{\partial R_n^{\kappa,k+1}}{\partial x_i} \bigg|_p (x_{i,p+1} - x_{i,p}) = R_n^{\kappa,k+1}(x_{i,p}) \quad (4.2.2.6)$$

All terms $\partial R_n / \partial x_i$ in the Jacobian matrix are evaluated by numerical differentiation. Eq. (4.2.2.8) is solved by sparse direct matrix methods (Duff, 1977) or iteratively by means of preconditioned conjugate gradients (Moridis and

Pruess, 1995). Convergence of the solution requires iteration until the residuals are reduced below a preset convergence tolerance

$$\left| \frac{R_{n,p+1}^{k,k+1}}{M_{n,p+1}^{k,k+1}} \right| \leq \varepsilon_1 \quad (4.2.2.7)$$

The default (relative) convergence criterion is $\varepsilon_1 = 10^{-5}$. When the accumulation terms are smaller than e_2 (default $e_2 = 1$), an absolute convergence criterion is imposed, $|R_n^{k,k+1}| \leq e_1 \cdot e_2$. Convergence is usually attained in 3 - 4 iterations. If convergence cannot be achieved within a certain number of iterations (the default is 8), the time step size Δt is reduced and a new iteration process begins.

The entire geometric information of the space discretization in Eq. (4.2.2.6) is provided in the form by grid block volumes V_n , interface areas A_{nm} , nodal distances D_{nm} and components g_{nm} of gravitational acceleration along nodal lines. There is no reference to a global system of coordinates, or to the dimensionality of a particular flow problem. The discretized equations are in fact valid for arbitrary irregular discretizations in one, two or three dimensions, and for porous as well as for fractured media. This flexibility should be used with caution because the accuracy of the solution depends upon the accuracy with which the various interface parameters in equation (4.2.2.3) and (4.2.2.4) can be expressed in terms of the average grid block condition. A general requirement is that approximate thermodynamic equilibrium exists in (almost) all grid blocks at (almost) all times (Pruess and Narasimhan, 1985). In systems of regular grids, the IDF formulation of Eq. (4.2.2.6) is identical to a conventional finite difference scheme (Peaceman, 1977).

4.2.3 Options of EOS Modules

The thermophysical properties of the fluid mixtures in the governing mass- and energy-balance equations are provided by equation-of-state (EOS) modules which determine the number of phases and components considered by the model.

The EOS module computes all secondary (thermophysical) parameters as functions of the primary variables. Furthermore, the following diagnosis is performed:

- 1) the phase conditions in each element has to be recognized depending on the given set of primary variables,
- 2) the appearance and disappearance of phases must be diagnosed as primary variables change during the Newton-Raphson iteration process, and
- 3) primary variables must be switched in response to a phase change.

In TOUGH2, all secondary parameters used in the flow equations are calculated as a function of a limited set of primary variables. This concept provides maximum flexibility in the choice of primary variables. Each EOS module has its own set of primary variables which furthermore depends on the phase composition in each element of the model.

EOS1 (Water, Water with Tracer): This is the most basic EOS module. It provides the thermodynamic properties of pure water in its liquid, vapor, and two-phase states. In addition, two waters of identical physical properties can be distinguished by a trace component. All water properties (density, specific enthalpy, viscosity, saturated vapor pressure) are calculated from the steam table equations as given by the International Formulation Committee (1967).

EOS2 (Water, CO₂): This fluid property module was developed by O'Sullivan et al. (1985) to describe fluids in gas-rich geothermal reservoirs, which often contain CO₂ mass fractions ranging from a few percent to over 80% (Atkinson et al., 1980). It accounts for the non-ideal behavior of gaseous CO₂, and the dissolution of CO₂ in the aqueous phase according to Henry's law with heat-of-solution effects. The thermophysical property correlations are based on the model of Sutton and McNabb (1977); a formulation from Pritchett et al. (1981) is used for the viscosity of vapor-CO₂ mixtures.

EOS3 (Water, Air): This module is an adaptation of the EOS module of TOUGH, and implements the same thermophysical properties model (see Pruess, 1987). All water properties are represented by the steam table equations (International Formulation Committee, 1967). Air is approximated as an ideal gas, and additivity is assumed for air and vapor partial pressures in the gas phase, i.e. $P_g = P_a + P_v$. The viscosity of air-vapor mixtures is computed from a formulation according to Hirschfelder et al. (1954). The solubility of air in liquid water is represented by Henry's law, i.e., the dissolved air mole fraction $X_1^{(air)}$ is proportional to the air partial pressure in the gas phase. EOS3 is the most frequently used EOS module of TOUGH2 for simulating fluid flow and thermal loading at Yucca Mountain.

EOS4 (Water, Air, with Vapor Pressure Lowering Capability): This EOS differs from EOS3 in that provision is made for vapor pressure lowering effects. Vapor pressure is expressed by Kelvin's equation (Edlefsen and Anderson, 1943), and depends not only on temperature, but also on capillary pressure.

EOS5 (Water, Hydrogen): This property module was developed to study the behavior of groundwater systems in which hydrogen release occurs. It is related to EOS3, the main difference being that the air component is replaced by hydrogen, which has different thermophysical properties.

4.2.4
Boundary Condition
Treatment

In TOUGH2, boundary conditions are generally specified by means of appropriately chosen volume elements, flow connections, and sinks (pumping wells) and sources (injection wells). Boundary conditions can be of two basic types. Dirichlet conditions prescribe constant thermodynamic conditions, such as pressure or temperature on the boundary, while Neumann conditions prescribe fluxes of mass or heat crossing boundary surfaces. A special case of a Neumann boundary condition is "no flux", which in the integral finite difference framework is handled by not specifying any flow across the boundary. More general flux conditions are prescribed by introducing sinks or sources of appropriate strengths into the elements adjacent to the boundaries.

Dirichlet-type boundary conditions, such as constant pressures or temperatures, can be specified by introducing appropriate boundary elements and connections. A connection consists of an interface area, and a pair of adjacent nodes at some distance from the interface. Assigning very large volumes to Dirichlet-type boundary elements will ensure that their thermodynamic state remains unchanged during a simulation. It is also possible to maintain a constant temperature and to allow pressure to vary by assigning a very large heat capacity to an element with "normal" volume. The only feature distinguishing boundary elements from the "normal" grid blocks in the interior of the flow domain is their large volume (and/or heat capacity); in the calculations they can be ignored or treated in the same way as any other element.

TOUGH2 can implement Dirichlet conditions by using the concept of "active" and "inactive" elements. By convention, elements in the data block ELEME (or files MESH or MINC) are considered "active" until the first element entry with a zero or negative volume is encountered. All subsequent elements are considered inactive. For the inactive elements no mass or energy balance equations are set up, and their primary thermodynamic variables are not included in the vector of the unknowns. Inactive elements may appear in flow connections and initial condition specifications like all other elements.

This feature can be used to specify Dirichlet boundary conditions by gathering all elements beyond the desired flow domain boundary at the end of the ELEME block and inserting a dummy volume element of zero volume in front of them. Thermodynamic conditions for the inactive elements are maintained as initially prescribed during a simulation run.

The specification of inactive elements can also be used in the MESH-MAKER module to steer the MINC-process of subgridding volume elements. By convention, inactive elements will remain unpartitioned, i.e., they will be treated as a single porous medium.

4.2.5
Treatment of
Fractured/Matrix Flow and
Interaction

TOUGH2 is designed for the simulation of multi-phase, multi-component, and heat flow in porous and fractured media. In flow through fractured porous media, the key issue is how to evaluate fluid exchange between matrix blocks and the surrounding fractures. The available methods include: (1) an explicit discrete fracture and matrix treatment; (2) the effective continuum method (ECM); (3) the dual-porosity method; (4) the dual-permeability method; and (5) the multiple interacting continua (MINC) method (Pruess and Narasimhan, 1985). All these options for the treatment of fracture and matrix flow are available in the TOUGH2 code.

Figure 4.2.2 illustrates the classical dual-porosity concept for modeling flow in fractured-porous media as developed by Warren and Root (1963). The flow domain is composed of matrix blocks of low permeability, embedded in a network of inter-connected fractures. Global flow in the reservoir occurs only through the fracture system, which is described as an effective porous continuum. Rock matrix and fractures may exchange fluid (or heat) locally by means of "interporosity flow," which is driven by the difference in pressures (or temperatures) between matrix and fractures. Warren and Root (1963) approximated the interporosity flow as being "quasi-steady," with the rate of matrix-fracture interflow proportional to the difference in (local) average pressures.

Figure 4.2.2
Idealized "double porosity" model of a fractured porous medium.

The "quasi-steady" approximation is applicable to isothermal single-phase flow of fluids with small compressibility and large pressure diffusivities (mainly liquids), in which pressure changes in the fractures are propagated rap-

idly into the matrix blocks. However, for multiphase flow or coupled fluid and heat flow, the transient periods for interporosity flow can be very long (tens of years). In order to accurately describe such flows, it is necessary to resolve the driving pressure, temperature and mass fraction gradients at the matrix/fracture interface. In the method of "multiple interacting continua" (MINC; Pruess and Narasimhan, 1982, 1985), resolution of these gradients is achieved by appropriate subgridding of the matrix blocks, as shown in Figure 4.2.3.

The MINC concept is based on the notion that changes in fluid pressures, temperatures, phase compositions, etc. due to the presence of sinks and sources (production and injection wells) will propagate rapidly through the fracture system, while invading the tight matrix blocks only slowly. Therefore, changes in matrix conditions will (locally) be controlled by the distance from the fractures. Fluid and heat flow from the fractures into the matrix blocks, or from the matrix blocks into the fractures, can then be modeled by means of one-dimensional strings of nested grid blocks, as shown in Fig. 4.2.3.

Figure 4.2.3

Subgridding in the method of "multiple interacting continua" (MINC).

In general it is not necessary to explicitly consider subgrids in all of the matrix blocks separately. Within a certain reservoir subdomain (corresponding to a finite difference grid block), all fractures will be lumped into continuum #1, all matrix material within a certain distance from the fractures will be lumped into continuum #2, matrix material at a larger distance becomes continuum #3, and so on. Quantitatively, the subgridding is specified by means of a

set of volume fractions $VOL(j)$, $j = 1, \dots, J$, into which the "primary" porous medium grid blocks are partitioned.

The MINC-process in the MESHPMAKER module of TOUGH2 operates on the element and connection data of a porous medium mesh to calculate, for given data on volume fractions, the volumes, interface areas, and nodal distances for a "secondary" fractured medium mesh. The information on fracturing (spacing, number of sets, shape of matrix blocks) required for this is provided by a "proximity function" $PROX(x)$ which expresses, for a given reservoir domain V_o , the total fraction of matrix material within a distance x from the fractures. If only two continua are specified (one for fractures, one for matrix), the MINC approach is reduced to the conventional dual-porosity method. Full details are given in a separate report (Pruess, 1983a).

The MINC-method as implemented in the MESHPMAKER module can also describe global matrix-matrix flow, in addition to fracture-fracture connections. Figure 4.2.4 shows the most general approach, often referred to as "dual permeability," in which global flow occurs in both fracture and matrix continua. It is also possible to permit matrix-matrix flow only in the vertical direction. For any given fractured reservoir flow problem, selection of the most appropriate gridding scheme must be based on a careful consideration of the physical and geometric conditions of flow. The MINC approach is not applicable to systems in which fracturing is so sparse that the fractures cannot be approximated as a continuum. More details about MINC are given Chapter 6 (Doughty, et al., 1996).

Figure 4.2.4

Flow connections in the "dual permeability" model. Global flow occurs between both fracture (F) and matrix (M) grid blocks. In addition there is F-M interporosity flow.

4.3 ITOUGH2

4.3.1 Introduction

ITOUGH2 (Inverse TOUGH2) is a computer program that provides inverse modeling capabilities for the TOUGH2 code. While the main purpose of ITOUGH2 is to estimate model-related hydraulic properties by calibrating TOUGH2 models to laboratory or field data, the information obtained by evaluating parameter sensitivities can be used to optimize the design of an experiment, and to analyze the uncertainty of model predictions.

ITOUGH2 solves the inverse problem by automatic model calibration based on the maximum likelihood approach. All conceivable TOUGH2 input parameters can be considered unknown or uncertain. The parameters are estimated based on any type of observations for which a corresponding TOUGH2 output is available, including prior information about the parameters to be estimated. A number of different objective functions and minimization algorithms are available. One of the key features of ITOUGH2 is its extensive error analysis, which provides statistical information about residuals, estimation uncertainties, and the ability to discriminate among model alternatives. The impact of parameter uncertainties on model predictions can be studied by means of linear error analysis or Monte Carlo simulations.

The procedure of inverse modeling is summarized in Table 4.3.1.1 and visualized in Figure 3.1.1, in which the process of iteratively updating model parameters to improve the match of observed data is described. The key elements of an inverse modeling code are (1) the simulation program to model the flow and transport in the hydrogeologic system, (2) the objective function which measures the deviation between the model output and the data, (3) the minimization algorithm which reduces the objective function by automatically updating parameter values, and (4) the error analysis which allows the evaluation of the quality of the inverse modeling results.

Computer Models and their Development for the Unsaturated Zone Model at Yucca Mountain

Table 4.3.1.1 Stepwise procedure of parameter estimation by inverse modeling		
Step	Element	Comment
1	model conceptualization	Develop a TOUGH2 model that simulates the experiment.
2	prior information	Select reasonable initial parameter values
3	simulation	Calculate system response
4	objective function	Compare observed and calculated system state
5	minimization algorithm	Update parameters so that the value of the objective function decreases
6	iteration / convergence	Repeat step 3-5 until no further improvement of the fit can be achieved
7	error analysis	Perform sensitivity and residual analysis, calculate estimation uncertainty and parameter correlations, calculate model identification criteria, perform model test, calculate prediction error

The core of ITOUGH2 is any of the modules of the TOUGH2 family of codes. The first version, named ITOUGH (Finsterle, 1992), was based on the TOUGH code (Pruess, 1987). It was then adapted to the architecture of TOUGH2 (Pruess, 1991) with its flexible array structure. This version is documented in Finsterle (1993). ITOUGH2 has been continuously updated to accommodate new TOUGH2 modules such as T2CG1 (Moridis and Pruess, 1995), T2VOC (Falta et al., 1995), or new equation-of-state (EOS) modules, such as the Effective Continuum Model (ECM) described in Chapter 6 (Doughty et al. 1996). Furthermore, new parameter and observation types as well as program options have been added as needed. The program architecture of ITOUGH2 allows for a flexible adaptation of the inverse code to any modification of the simulation program TOUGH2 and its derivatives. ITOUGH2 also provides an interface for specifying problem-dependent parameters and observations. This flexibility significantly increases the applicability of the code to a variety of problems for which an inverse solution is sought.

ITOUGH2 underwent software qualification according to the YMP-LBL General Software Quality Assurance procedure (Wu et al., 1996).

Figure 4.3.1.1
Inverse modeling flow chart.

4.3.2 Methodology

The ITOUGH2 code solves the inverse problem by automatic model calibration based on an indirect approach (Carrera and Neuman, 1986) which makes use of optimization techniques. It is important to realize that efficient and stable solution of the direct problem, i.e. the simulation of multiphase fluid and heat flow in fractured-porous media, is a key step in inverse modeling. This task is fulfilled by the TOUGH2 code. ITOUGH2 repeatedly performs TOUGH2 simulations, and compares the results with available data. Based on this comparison, improved estimates of model parameters can be made.

In this report we develop the methodology of inverse modeling in general terms. However, we restrict ourselves on those features that are actually implemented in the ITOUGH2 code. While ITOUGH2 provides a detailed residual and error analysis including error propagation analysis, we only discuss the basic concepts in this report (for more details see Finsterle, 1993).

ITOUGH2 estimates elements of a parameter vector p based on observations summarized in a vector z by minimizing a weighted least-square objective function S using the Levenberg-Marquardt algorithm. The vector p of length n contains the parameters to be estimated by inverse modeling. The parameters have to be TOUGH2 input parameters or a (user-specified) function thereof. Ele-

ments of vector $\mathbf{p}$ may include hydrogeologic properties (such as absolute permeability, a parameter of the capillary pressure or relative permeability function), initial and boundary conditions, or geometrical features such as fracture spacing which is an input parameter of the MINC preprocessor.

Vector $\mathbf{z}$ of length m contains dependent, observable variables at discrete points in space and time (= calibration points). The elements of $\mathbf{z}$ represent those state variables for which both an observed value (i.e. measured data point) and a corresponding TOUGH2 output is available. The most commonly used observations for calibration are pressures, flow rates, temperature and concentration measurements. The vector of observable variables may also contain measured parameter values. For example, if permeability has been measured on cores in the laboratory, this information can be considered as an additional data point, and treated along with the direct observations of the system response. Such measured parameter values are referred to as "prior information".

The residual vector $\mathbf{r}$ contains the differences between the measured and calculated system response:

$$\text{Residual vector} \quad \mathbf{r} = \mathbf{z} - \hat{\mathbf{z}} \quad (4.3.2.1)$$

For example, r_1 is the difference between the measured and calculated pressure at a certain point in space and time. A special type of residuals are the differences between the measured parameters (prior information) and the estimated parameter values. This difference - appropriately weighted - can be used as a plausibility criterion to judge the inversion.

Next we try to relate the residual to the measurement error. Consider a dataset that is drawn from a true, but unknown system response $\mathbf{z}$ (see Figure 4.3.2.1). The individual measurement error is defined as the difference between the measured and the true value, $(z^* - z)$. The modeling error is defined as the difference between the true and the calculated system response, $(z - \hat{\mathbf{z}})$. Since the true system response $\mathbf{z}$ is unknown, neither the measurement nor the modeling errors are known. However, we can try to describe them in statistical terms by assuming that they follow a certain distribution. Furthermore, the difference between the measured and the modeled quantities (i.e. the residuals) can be calculated. Note that the aim of inverse modeling is to provide an estimate of the true system behavior. If the true values were identified, the residuals are equal to the measurement errors. In other words, the statistical characteristics of the residuals should be similar to the ones of the measurement errors.

Figure 4.3.2.1

True, measured, and calculated system response, definition of measurement and modeling error.

The unexplained part (e.g. measurement errors) of the system response cannot be described individually, but by means of a stochastic model. A reasonable assumption about the measurement errors is that they are uncorrelated, normally distributed random variables with zero mean (the residual analysis will have to show whether this assumption was justified). The distributional assumption can therefore be summarized in a covariance matrix C_{zz} . C_{zz} is an $m \times m$ diagonal matrix. The i -th diagonal element of matrix C_{zz} is the variance σ_i^2 representing the measurement error of observation z_i .

$$C_{zz} = \begin{bmatrix} \sigma_1^2 & 0 & 0 & 0 & \cdots & 0 \\ 0 & \sigma_i^2 & 0 & 0 & \cdots & 0 \\ 0 & 0 & \sigma_n^2 & 0 & \cdots & 0 \\ 0 & 0 & 0 & \sigma_j^2 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & \sigma_m^2 \end{bmatrix} \quad (4.3.2.2)$$

The objective function S is a measure of the misfit between the data and the model calculation. If the measurement errors $(z^* - z)$ are normally distributed with mean $E((z^* - z)) = 0$ and covariance matrix $E((z^* - z)(z^* - z)^T) = C_{zz}$, maximum-likelihood theory yields the following objective function to be minimized:

$$S = (z^* - \hat{z}(p)) C_{zz}^{-1} (z^* - \hat{z}(p))^T = r^T C_{zz}^{-1} r \quad (4.3.2.3)$$

Minimizing the objective function (4.3.2.3) can be performed by local linearization and setting the derivative of S with respect to p to zero. This leads to the Jacobian matrix J of dimensions $m \times n$, the elements of which are defined as follows:

$$J_{ij} = -\frac{\partial r_i}{\partial p_j} = \frac{\partial z_i}{\partial p_j} \quad (4.3.2.4)$$

ITOUGH2 calculates the Jacobian using either forward or centered finite differences.

The Levenberg-Marquardt modification of the Gauss-Newton algorithm is a rather general and robust procedure for iteratively updating the parameter vector p (Levenberg, 1944; Marquardt, 1963). It can be described as follows (Table 4.3.2.1):

Table 4.3.2.1 Levenberg-Marquardt algorithm

$$\Delta p = (J^T C_{zz}^{-1} J + \lambda D)^{-1} J^T C_{zz}^{-1} r \quad (4.3.2.5)$$

$$p^{(k+1)} = p^{(k)} + \Delta p \quad (4.3.2.6)$$

decrease λ by factor v if $S(p^{(k+1)}) < S(p^{(k)})$

increase λ by factor v if $S(p^{(k+1)}) > S(p^{(k)})$

λ = Levenberg parameter ($\lambda^{(k=0)} \approx 0.001$)

v = Marquardt parameter ($v \approx 10$)

D = Diagonal matrix with $D_{ii} = (J^T C_{zz}^{-1} J)_{ii}$

If λ is large, the first term on the right-hand side of (4.3.2.5) becomes a matrix which has a dominant diagonal. This leads to a small step along the gradient of S . Stepping along the steepest descent direction is robust, but inefficient. With decreasing values for the Levenberg parameter, (4.3.2.5) converges to the Gauss-Newton algorithm with its quadratic convergence rate.

One of the key advantages of a formalized approach to parameter estimation is the possibility to perform an extensive *a posteriori* error analysis. First, the

residual analysis provides some measure of the overall goodness-of-fit. Next we can determine the uncertainty of the estimated parameters. Note that a good match does not necessarily mean that the estimates are reasonable. They may be highly uncertain due to high parameter correlation (an indication of over-parameterization). The covariance matrix of the estimated parameters can be further analyzed to obtain correlation coefficients, eigenvalues and eigenvectors, which describe parameter combinations that lead to similar matches, etc. Finally, we can calculate the uncertainty of the simulation results, which also allows us to identify potential outliers in the data.

The estimated error variance represents the variance of the mean weighted residual and is thus a measure of goodness-of-fit:

$$s_0^2 = \frac{\mathbf{r}^T \mathbf{C}_{zz}^{-1} \mathbf{r}}{m - n} \quad (4.3.2.7)$$

Note that if the residuals are consistent with the distributional assumption about the measurement errors (i.e. matrix $\mathbf{C}_{zz}$), then the estimated error variance assumes a value close to one. Next we calculate the expected value and the covariance matrix $\mathbf{C}_{pp}$ of the estimated parameters. Based on the linearity assumption it can be shown that the expected value of the estimated parameter is equal to the parameter itself. The definition of a covariance matrix yields:

$$\mathbf{C}_{pp} = s_0^2 \cdot (\mathbf{J}^T \mathbf{C}_{zz}^{-1} \mathbf{J})^{-1} \quad (4.3.2.8)$$

The Jacobian $\mathbf{J}$ is evaluated at the optimum parameter set. The interpretation of the covariance matrix $\mathbf{C}_{pp}$ provides the key criteria to evaluate the inverse modeling results. The elements of matrix $\mathbf{C}_{pp}$ are directly proportional to the overall goodness-of-fit expressed by s_0^2 . The diagonal elements of $\mathbf{C}_{pp}$ contain the variances $\sigma_{p_i}^2$ of the estimated parameters. The off-diagonal terms are the covariances c_{ij} . Correlation among parameters can be described as a conjoint impact of parameter changes on the system behavior. The correlation coefficient is given by:

$$r_{ij} = \frac{c_{ij}}{\sqrt{\sigma_i^2 \cdot \sigma_j^2}} \quad (4.3.2.9)$$

The correlation coefficient assumes values between -1 and 1; a value of zero indicates no statistical correlation between parameter i and j , a value close to -1 or 1 indicates strong correlation, i.e. the two parameters cannot be determined independently. Even though certain pairs of parameters may exhibit a preferential correlation structure, correlations are not invariable entities of parameter combinations. They obviously depend on the available data, and also on the number of simultaneously estimated parameters, since indirect correlations

may overwhelm the direct correlations. If correlations exist, the uncertainty of one parameter does affect the uncertainty of the other parameter. The diagonal elements of matrix C_{pp} , which are the variances from the joint probability density function, account for this fact. They have to be distinguished from the conditional or marginal standard deviation $\sigma_{p_i}^*$ which measures the uncertainty of a parameter assuming that all the other parameters are either exactly known or uncorrelated. The marginal standard deviation is obviously always smaller than the one from the joint probability density function. The situation is illustrated in Figure 4.3.2.2 for the case of two parameters. The ratio

$$\chi_i = \frac{\sigma_{p_i}^*}{\sigma_{p_i}} \quad (4.3.2.10)$$

is a measure of how independently parameter i can be estimated. Small values of χ_i usually indicate that the uncertainty σ_{p_i} of a parameter could be reduced by lowering its correlation to other parameters.

Figure 4.3.2.2
Confidence region, joint and conditional standard deviation

As mentioned earlier, maximum likelihood estimation leads to optimum parameters for a given model structure. However, this does not imply that the true system behavior has been identified. If the conceptual model fails to reproduce the salient features of the groundwater system, the calibrated model may not be able to match the observed data as expected (note that our expectation regarding the fit is reflected in the *a priori* covariance matrix C_{zz}). A statistical test of the random variable s_n^2 / σ_n^2 gives a first indication of whether the model fits

the data well enough so that the underlying conceptual model can be accepted. More details about the error analysis can be found in *Finsterle* (1993) and *Finsterle and Pruess* (1995).

4.3.3 Applicability of ITOUGH2

The architecture of ITOUGH2 is such that any conceivable TOUGH2 input parameter can be estimated based on any observable variable, for which a corresponding TOUGH2 output can be calculated. This flexibility of the code makes it suitable for a wide range of applications.

A limitation is the fact that the evaluation of the Jacobian matrix is performed numerically by means of the perturbation method. This requires solving the forward problem as many times as the number of parameters to be estimated. As a result, ITOUGH2 inversions can be very expensive in terms of CPU-time.

It should also be realized that parameter estimation by inverse modeling is based on the assumption that the conceptual model is correct. Systematic errors in either the data or the model lead to biased estimates. Furthermore, the inverse problem can be ill-posed, i.e. the solution is non-unique or unstable due to a lack of sensitive data, high correlation coefficients because of over parameterization, or noise in the data.

While these problems are the most important and difficult ones in inverse modeling, they are not limitations of ITOUGH2. In fact, ITOUGH2 provides a number of measures to identify flaws in the data and the model. This information can also be used to optimize the design of future experiments.

ITOUGH2 has been applied to problems pertinent to the Yucca Mountain Project. The estimation of two-phase hydrogeologic properties for the LBNL-USGS 3D Site Scale Model of the unsaturated zone at Yucca Mountain is an example that demonstrates the use of inverse modeling techniques for the determination of model-related parameters under consideration of prior information. Permeability, parameters of the characteristic curves, thermal properties, as well as boundary conditions such as infiltration rates have been determined based on a variety of observations such as pressures, gas flow rates, saturations, water potentials, and temperatures. The error analysis provided insight into estimation uncertainties, parameter correlations, and the sensitivity of the system with respect to individual parameters.

The applicability of ITOUGH2 to a variety of problems in nuclear waste isolation, geothermal field performance, and aquifer remediation has been documented in a number of articles. A list of references can be found in *Wu et al.* (1996).

4.4 Rautman's Thermal Conductivity Model

A thermal conductivity model, developed by Rautman (1995a and 1995b), has been implemented into the TOUGH2 code for studies of geothermal and thermal loading conditions at Yucca Mountain. Rautman's model was derived from spatially correlated, surrogate material-property models of porosity, using a multiple linear-regression equation. This model expresses thermal conductivity as a function of porosity, temperature and liquid saturation for the tuffs at Yucca Mountain. Multiple linear regression analyses of thermal conductivity values against porosity and the various initial test conditions indicate that the relationship is of the form (Rautman, 1995a and 1995b):

$$k_t = C_0 + C_1 T + C_2 S + C_3 \phi \quad (4.4.1)$$

where k_t is the thermal conductivity (W/m °C), T is the temperature (°C), S is the liquid saturation, and ϕ is the porosity.

Different coefficients are used for welded and nonwelded tuffs at Yucca Mountain. They are given in Table (4.4.1).

Table 4.4.1 Coefficients of Multiple Linear Regressions Relating Thermal Conductivity (Rautman, 1995b)				
Coefficient	Low Temperature, $T \leq 100^\circ\text{C}$		High Temperature, $T > 100^\circ\text{C}$	
	Welded	Nonwelded	Welded	Nonwelded
C_0	1.748	1.250	1.916	1.039
C_1	3.529×10^{-4}	2.096×10^{-3}	1.564×10^{-4}	3.370×10^{-4}
C_2	0.4347	0.5853	0	0
C_3	-3.210	-2.238	-4.055	-1.530

4.5 Effective Continuum Approach

A key issue in modeling studies of moisture movement in the Yucca Mountain is the evaluation of fracture-matrix flow. The ECM approach has recently found wide applications in the Yucca Mountain site characterization studies because of its simplicity in terms of data requirements and computational efficiency. The effective continuum approach can accommodate two-phase flow in a fracture-matrix system, and is based on the assumption that local thermodynamic equilibrium exist between the fracture and matrix system (Pruess et. al., 1990a and b).

Two types of ECM formulation have been implemented in our studies of moisture, gas and heat flow at the mountain. The first is referred as to the generalized ECM formulation, and the second method uses a threshold saturation fracture flow model. The two methods are discussed in this section.

4.5.1
Generalized Effective
Continuum Approach

The generalized ECM formulation (Pruess, 1985) is based on the assumption that there is approximate thermodynamic equilibrium (locally) between fracture and matrix at all times in the formation. If we consider single-component two-phase flow in a fractured porous medium, the conditions for thermodynamic equilibrium in the ECM formulation are:

(a) equality of temperatures:

$$T_m \approx T_f \quad (4.5.1.1)$$

and (b) equality of pressures:

$$P_{\beta,m} \approx P_{\beta,f} \quad (4.5.1.2)$$

where the subscript m and f denote matrix and fracture, respectively, and β indicates the phase ($\beta=l$: liquid, $\beta=g$: gas).

Under such equilibrium conditions, we will have the same capillary pressures

$$P_{c,m} \approx P_{c,f} \quad (4.5.1.3)$$

the same densities

$$\rho_{\beta,m} \equiv \rho_{\beta,f} \quad (4.5.1.4)$$

and the same viscosities

$$\mu_{\beta,m} \equiv \mu_{\beta,f} \quad (4.5.1.5)$$

for the matrix and fracture continuum, respectively.

Darcy's law for single-component two-phase flow in a fractured porous medium can be written in the following form,

$$F_{\beta, \text{matrix}} = -k_m k_{\beta, m} \left(\frac{\rho_{\beta}}{\mu_{\beta}} \right)_m (\nabla P_{\beta, m} - \rho_{\beta, m} \mathbf{g}) \quad (4.5.1.6)$$

$$F_{\beta, \text{fractures}} = -k_f k_{\beta, f} \left(\frac{\rho_{\beta}}{\mu_{\beta}} \right)_f (\nabla P_{\beta, f} - \rho_{\beta, f} \mathbf{g}) \quad (4.5.1.7)$$

where Φ = mass flux;

k_m (k_f)= equivalent single-phase continuum permeability of matrix (fractures);

$k_{\beta, m}$ ($k_{\beta, f}$)= relative permeability to phase β in matrix (fractures);

ρ_{β} = density of phase β

μ_{β} = viscosity of phase β

P_{β} = pressure of phase β

$\mathbf{g}$ = acceleration of gravity

Under conditions of (local) thermodynamic equilibrium we have the following expression for total flux:

$$F_{\beta} = F_{\beta, m} + F_{\beta, f} = -(k_m k_{\beta, m} + k_f k_{\beta, f}) \frac{\rho_{\beta}}{\mu_{\beta}} (\nabla P_{\beta} - \rho_{\beta} \mathbf{g}) \quad (4.5.1.8)$$

Note that equality of pressures implies equality of pressure gradients. In (4.5.1.8), the relative permeabilities $k_{\beta, m}$ and $k_{\beta, f}$ have to be evaluated at saturations $S_{\beta, m}$ and $S_{\beta, f}$, respectively, such that $P_{c, m}(S_{\beta, m}) = P_{c, f}(S_{\beta, f})$.

The expression for total flux can be interpreted as referring to a single effective continuum with total effective phase permeability of $k_m k_{\beta, m} + k_f k_{\beta, f}$. For single phase flow, the effective continuum permeability becomes $k = k_m + k_f$, so

that the effective continuum relative permeability to phase β can be defined as

$$k_{\beta} = \frac{k_m k_{\beta,m} + k_f k_{\beta,f}}{k_m + k_f} \quad (4.5.1.9)$$

The total phase flux is then given by the following single continuum expression

$$F_{\beta} = -k_{\beta} \frac{\rho_{\beta}}{\mu_p} (\nabla P_{\beta} - \rho_{\beta} g) \quad (4.1.10)$$

In these equations we have defined relative permeabilities relative to total single phase permeability, so that $0 \leq k_{\beta} \leq 1$.

The numerical implementation of the ECM scheme is straightforward once the liquid saturations in the matrix and fracture are known. This can be achieved by introducing a fracture-matrix composite capillary pressure curve, which is based on the individual fracture and matrix capillary pressure curves. Under local equilibrium conditions, the combined P_c curve is

$$P_c(S_l) = P_{c,m}(S_{l,m}) = P_{c,f}(S_{l,f}) \quad (4.5.1.11)$$

where $S_{l,m}$ and $S_{l,f}$ is the liquid saturation in the fracture and matrix continuum, respectively, and S_l is the combined saturation which is a function of a combined or average liquid saturation:

$$S_l = \frac{S_{l,m} \phi_m + S_{l,f} \phi_f}{\phi_m + \phi_f} \quad (4.5.1.12)$$

TOUGH2 solves for the combined saturation S_l . This saturation value can be used in the combined P_c curve to calculate the combined capillary pressure, which is the same for the fracture and the matrix continuum. The fracture and matrix saturations can then be determined by inverting the P_c functions of the fracture and the matrix, respectively. The ECM relative permeabilities are evaluated as follows:

$$k_{rl}^i = \frac{k_m^i k_{rl,m}(S_{l,m}) + k_f^i k_{rl,f}(S_{l,f})}{k_m^i + k_f^i} \quad (4.5.1.13)$$

The superscript i denotes the principal direction ($i=1, 2$, and 3), which allows the use of anisotropic permeabilities.

4.5.2 Threshold Saturation Fracture Flow ECM Formulation

In the effective-continuum approximation (Pruess and Tsang, 1994), the capillary pressure P_c and the equivalent continuum permeabilities to the liquid and gas phase (k_l and k_g), respectively, are expressed in terms of the continuum liquid saturation S_l .

4.5.2.1 Threshold Liquid Saturation

Let S_l be the liquid saturation of the effective continuum. It is expressed in terms of the matrix and fracture saturations as follows (Pruess et al., 1988):

$$S_l = \frac{S_{lm} \phi_m + S_{lf} \phi_f}{\phi_m + \phi_f} \quad (4.5.2.1)$$

where both ϕ_m and ϕ_f are the porosities of the matrix and the fractures, respectively, defined in terms of the total volume (V_{tot}),

$$V_{tot} = V_m + V_f \quad (4.5.2.2)$$

and S_{lm} and S_{lf} are liquid saturations in matrix and fractures, respectively. In Equation (4.5.2.2) V_m and V_f are matrix and fracture volumes.

A threshold saturation S_{th} is defined as the continuum liquid saturation at the juncture when the matrix is fully saturated and the fracture is dry (Pruess and Tsang, 1994). S_{th} is obtained from Equation (4.5.2.1) when S_{lm} is 1 and S_{lf} is 0.

$$S_{th} = \frac{\phi_m}{\phi_m + \phi_f} = 1 - \frac{\phi_f}{\phi} \quad (4.5.2.3)$$

with

$$\phi = \phi_m + \phi_f$$

The effective-continuum concept is only applicable when approximate local thermodynamic equilibrium exists between matrix and fractures. Because the capillary suction in the matrix is much stronger than that in the fracture, local equilibrium implies that the liquid saturation in the fracture will remain near zero until matrix saturation approaches 100%. The concept of a threshold continuum saturation (Equation 4.5.2.3) is based on the assumption that the large disparity of the capillary pressures in the matrix and fractures will cause (a) the fractures to remain dry until the matrix becomes fully saturated during imbibition.

tion, and (b) the fractures to be completely drained before the matrix begins to desaturate during drainage.

From Equation (4.5.2.1), given the liquid saturation of the effective continuum, S_l , the matrix and fracture liquid saturation are evaluated as follows:

$$S_{lm} = S_l/S_{th}, \quad S_{lf} = 0 \quad ; \text{ for } S_l \leq S_{th} \quad (4.5.2.4)$$

$$S_{lm} = 1, \quad S_{lf} = \frac{S_l - S_{th}}{1 - S_{th}}; \text{ for } S_l > S_{th}$$

4.5.2.2 Capillary Suction

The capillary pressure for the effective continuum in terms of the continuum saturation is:

$$P_c(S_l) = P_c(S_{lm} - \delta) \quad \text{for } S_l < S_{th} \quad (4.5.2.5)$$

$$= P_c(1 - \delta) \frac{1 - S_l}{1 - S_{th}} \quad \text{for } S_l \geq S_{th}$$

The parameter δ is introduced to represent air entry effects, i.e., a finite suction is required to reduce the matrix saturation from $S_{lm} = 1$. Equation (4.5.2.5) results in a continuous curve as the continuum liquid saturation passes through the threshold value. Below the threshold level, it follows the suction curve for the matrix; above the threshold saturation, the capillary pressure in the fracture varies linearly with S_l .

4.5.2.3 Effective-Continuum Liquid and Gas Permeability

The effective-continuum liquid and gas permeabilities are defined as functions of the effective-continuum liquid saturation as well as in terms of the anisotropic permeabilities of the matrix and fractures.

For liquid permeabilities:

$$k_l^i(S_l) = k_e^i k_{rl}^i \quad (4.5.2.6)$$

where the total effective-continuum permeability in the principal direction ($i=1,2,3$) is defined by:

$$k_e^i = k_m^i + k_f^i \quad (4.5.2.7)$$

and k_m^i and k_f^i are the saturated matrix and fracture continuum permeabilities, respectively. The relative permeabilities in the principal direction i in Equation (4.5.2.6) are defined as:

$$\begin{aligned} k_{rl}^i &= \frac{k_m^i(1-\phi_f)k_{rm}(S_{lm})}{k_e^i} \quad \text{for } S_l \leq S_{lh} \\ &= \frac{k_m^i(1-\phi_f) + k_f^i k_{rf}(S_{lf})}{k_e^i} \quad \text{for } S_l > S_{lh} \end{aligned} \quad (4.5.2.8)$$

In Equation (4.5.2.8), $k_{rm}(S_{lm})$ and $k_{rf}(S_{lf})$ are relative liquid permeabilities in the matrix and fracture systems, respectively, and are determined as functions of S_{lm} and S_{lf} , according to Equation (4.5.2.4).

Assuming that gas and liquid relative permeabilities sum to 1, the effective-continuum gas permeability may be expressed as the difference between the saturated permeability of the effective continuum and the permeability to the liquid phase. In each principal direction i :

$$k_g^i(S_l) = k_e^i - k_{rl}^i \quad (4.5.2.9)$$

where the gaseous phase relative permeabilities are

$$k_{rg}^i = \frac{k_m^i(1-\phi_f) + k_f^i - k_{rl}^i(S_l)}{k_e^i} \quad (4.5.2.10)$$

Here the effective-continuum phase relative permeabilities k_{rl}^i and k_{rg}^i are normalized by the total effective-continuum permeabilities of Equation (4.5.2.7).

4.6 Discussion of Modeling Issues

As a general purpose simulator, the TOUGH2 code offers many options and flexibilities in treating different situations and scenarios for multiphase, multi-component flow, and heat transport in soils and rocks. There is a wide range of potential multiphase fluid and heat flow problems, and caution must be exercised in applying a specific scheme or special feature of the code. At Yucca Mountain we are dealing with a highly heterogeneous fractured-porous geological system which consists of many layers of alternating welded and nonwelded units with large contrasts in (a) the degree of fracturing, and (b) matrix permeability and (c) porosity.

Two issues are discussed in this section. First, we examine the weighting scheme used to calculate mobilities at an interface between adjacent grid blocks. Secondly, we discuss the numerical treatment of the fracture-matrix interaction of the welded units.

4.6.1 Weighting Scheme for Mobilities

The selection of different weighting schemes for mobilities of fluids may have a significant impact on the simulation results. Caution must be exercised when dealing with rapid transient boundary conditions, such as in gas flow analysis. Using both 1-D rock columns from five observation boreholes and the 3-D site-scale model, we have conducted a series of preliminary studies to test all the options of permeability weighting schemes for gas flow simulations with the TOUGH2 code. The TOUGH2 weighting schemes include the following 6 options (summarized in Table 4.6.1.11):

Table 4.6.1 Options for different weighting schemes in TOUGH2.	
MOP(11)	Weighting Scheme
0	MOBILITIES ARE UPSTREAM WEIGHTED AND PERMEABILITY IS UPSTREAM WEIGHTED,
1	MOBILITIES ARE AVERAGED BETWEEN ADJACENT ELEMENTS AND PERMEABILITY IS UPSTREAM WEIGHTED,
2	MOBILITIES ARE UPSTREAM WEIGHTED AND PERMEABILITY IS HARMONIC WEIGHTED,
3	MOBILITIES ARE AVERAGED BETWEEN ADJACENT ELEMENTS AND PERMEABILITY IS HARMONIC WEIGHTED,
4	MOBILITY AND PERMEABILITY PRODUCT IS HARMONIC WEIGHTED,
5	MOBILITIES AND PERMEABILITY ARE AVERAGED BETWEEN ADJACENT ELEMENTS (NEW OPTION FOR THIS TESTING),
*where MOP(11) is an input parameter of TOUGH2.	

The simulated gas pressures from several 1-D discretization have been compared to the observed gas pressures in the Paintbrush nonwelded unit (PTn) and the Topopah Spring welded unit (TSw). We have found that good matches with observed data have been achieved using MOP(11)=3, 4 and 5. Moreover, the model gives similar solutions regardless of the degree of discretization used. The other options produce very different pressure responses. The differences in predicted gas pressures as a result of the chosen weighting schemes are (a) the use of relatively coarse grids in the site-scale model to represent the highly heterogeneous layered systems, and (b) the large contrasts in both permeability and relative permeabilities across interfaces of welded and nonwelded hydrogeologic units.

Water flow or infiltration effects on gas flow may be small at the site. Our sensitivity studies indicate that vertical saturation profiles are almost constant during the entire transient period to gas flow under different infiltration rates. Running the simulations using a two-phase mode, we determined that the behavior of gas flow may be very close to that of a single-phase flow regime. The weighting scheme with MOP(11)=4 is recommended for gas flow simulations at Yucca Mountain.

4.6.2 Treatment of Fracture and Matrix Flow

The key issue for simulating fluid and heat flow in the fractured welded units of the Yucca Mountain site is to evaluate fracture and matrix interactions under multi-phase, non-isothermal conditions. The available methods for treatment of fracture and porous matrix interactions using a numerical model include: (1) explicit discrete fracture and matrix model, (2) the ECM approach; (3) the dual porosity method, (4) the dual-permeability method, and (5) the more general (MINC) method (Pruess and Narasimhan, 1985). We have experimented with all of these options for treating fracture and matrix flow in our modeling studies of developing the unsaturated-zone flow model of Yucca Mountain. When applied to simulating moisture flow and heat transfer at the mountain, all these approaches require knowledge of fracture and matrix properties and their spatial distribution. These site-specific fracture/matrix parameters, however, are presently not well defined for many units of the tuffs at Yucca Mountain. Currently, only the effective-continuum approach has found wide applications because of its simplicity in terms of data requirement and computational efficiency in handling large model grids.

As implemented in the site-scale model with the TOUGH2 code (Wittwer et al., 1995), the two ECM models can both be used to simulate two-phase flow in a fracture-matrix system. However, it should be noted that the ECM method is based on the assumption that a local thermodynamic equilibrium exists between the fracture and matrix system, as discussed in Section 4.5. The limitation of this approximation should be examined for its use. When applicable, the ECM approach provides a substantial simplification of description of fluid and heat flow in fractured porous media. The favorable conditions for this method is when rock matrix blocks are relatively small and permeable, and fracture net-

work is relatively uniformly distributed. On the other hand, the ECM approximation may break down under certain unfavorable conditions, such as for very tight and low permeability rock matrix with rapid transient fracture flow, since it may take a long time to reach equilibrium conditions under such conditions.

At Yucca Mountain, the averaged net water infiltration rate into the unsaturated zone near the potential repository has been estimated to be low, less than 10 mm/yr. The moisture flow through the mountain is expected to be small and slow at most locations of the mountain. Therefore, the local hydraulic equilibrium between porous rock matrix and fractures may be a reasonable approximation to the moisture flow. As a result, the effective-continuum approach may provide reasonable simulation results for predicting the movement and the ambient hydrogeologic conditions. The continuum method will be particularly suitable for a situation when a long-term, averaged, or steady-state solution is sought. As concluded by Pruess et al. (1990b), the effective-continuum approximation will be applicable when "sufficiently" large space and time scales are considered. Both time and space discretizations in the three-dimensional site-scale unsaturated-zone model are relatively coarse, and the application of the continuum approach may be justified for the time and space scales of interest to the site-scale modeling studies. A detailed study of the different modeling approaches for simulating fracture-matrix interaction is given in Chapter 6 (Doughty et al., 1996).

4.7 Gas Flow Module

A gas flow module was developed for TOUGH2 to be used for efficient simulations of gas flow under partially saturated condition. The single-phase module uses the same description of the physical processes of multi-phase flow in saturated and unsaturated heterogeneous media as in standard TOUGH2. It provides an accurate description of gas flow dynamics and constitutive physical laws and properties affecting gas flow. It is capable of handling different geometries in one, two, and three dimensions, and rapidly changing surface atmospheric conditions. The only difference between the gas flow module and the standard version of TOUGH2 (Version 1.11, Pruess, 1996) is that the gas flow module solves only one conservation equation for the air component, i.e. the water mass and energy balance equations used in the standard TOUGH2 formulation are omitted.

The single-phase gas module takes into account the following physical processes (the governing equations are provided in Section 4.2). Only one mass balance equation (4.2.1.1) for the air component is set up. Flow of the gaseous phase occurs under pressure, viscous, and gravity forces according to Darcy's law, with interference between the phases represented by means of relative permeability functions. Mass-balance equations are written in integral form for an arbitrary flow domain. In addition, the formulation accounts for a simplified

description of Knudsen diffusion by means of a Klinkenberg factor for permeability (Knudsen, 1909; Klinkenberg, 1941; Hadley, 1982).

Liquid water and heat are assumed to be at steady state, but could be non-uniformly distributed within the system considered. The description of thermodynamic conditions is based on assumed local equilibrium of all phases.

The governing equations used in TOUGH2 gas flow module and their numerical implementation are applicable to one-, two-, or three-dimensional anisotropic porous or fractured media. As in standard TOUGH2, this module does not perform deformation analysis of the host medium and its effects on the multiphase flow behavior, but it allows for porosity changes in response to changes in pore pressure (compressibility) and temperature (expansivity).

The thermophysical properties of fluid mixtures needed in assembling the governing mass-balance equations are provided by the equation-of-state module EOS1G. It provides values for all secondary (thermophysical) parameters as functions of the primary variables. The EOS1G module is an adaptation of the EOS3 module of for the TOUGH2 program, and implements the same thermophysical properties model (see Pruess, 1987).

EOS1G differs from the EOS3 module of TOUGH2 in (a) that the only primary thermodynamic variable is the gas pressure, (b) the water phase is treated as a passive phase with stable distribution, and (c) temperature does not change. The system is assumed to be at two-phase conditions. Primary variables should be initialized identical to TOUGH2 (EOS3) specifications by setting $MOP(19) = 0$. A summary of EOS1G specifications is given in Table 4.7.1.

Table 4.7.1 Summary of EOS1G	
Components#1:	Air
Components#2:	Water
(NK, NEQ, NPH, NB)=	(1,1,1,8)
MOP(19)=	1

This gas flow module has been qualified for its use in the YMP studies (Wu et al., 1996).

4.8 Radionuclide Transport Module

A new module for simulating radionuclide transport in a general, 3-D, and irregular grid has been recently implemented into the TOUGH2 code. The objective of this module is to provide a numerical tool to handle radionuclide and tracer transport in a non-isothermal multi-phase flow environment, includ-

ing fracture-matrix interaction. The numerical method for this transport module is also based on the integral finite difference scheme, as in the TOUGH2 code.

The major assumptions of the radionuclide transport modules are (a) a radionuclide or a tracer exists and is transported only in the liquid phase, (b) transport mechanisms include molecular diffusion and hydraulic dispersion in the liquid phase in addition to advection, and (c) first order decay is taken into account. The radionuclide or tracer is introduced as an additional mass component into the standard TOUGH2 formulation

The work for documenting and benchmarking the new radionuclide transport module is underway and will be reported in a future report.

4.9 References

Ahlers, C.F., T.M. Bandurraga, G.S. Bodvarsson, G. Chen, S. Finsterle, and Y.S. Wu, Performance analysis of the LBNL/USGS three-dimensional unsaturated zone site-scale model, , Yucca Mountain Project Milestone 3GLM105M, Lawrence Berkeley National Laboratory, Berkeley, CA, 1995a.

Ahlers, C.F., T.M. Bandurraga, G.S. Bodvarsson, G. Chen, S. Finsterle, and Y.S. Wu, Summary of model calibration and sensitivity studies using the LBNL/USGS three-dimensional unsaturated zone site-scale model, Yucca Mountain Project Milestone 3GLM107M, Lawrence Berkeley Laboratory, Berkeley, CA, 1995b.

ACCN: MOL.19960208.0091-0097

DTN: LB092995312293.001 (Non-Q)

Atkinson P.G., R. Celati, R. Corsi, F. Kucuk, Behavior of the Bagnore steam/CO₂ Geothermal Reservoir, Italy, Soc. Pet. Eng. J., pp. 228-238, 1980.

Duff, I.S., MA28 - A Set of FORTRAN subroutines for sparse unsymmetric linear equations, AERE Harwell Report R 8730, 1977.

ACCN: NNA.19900614.0540

Edlefsen N.E., A.B.C. Anderson, Thermodynamics of soil moisture, Hilgardia, 15, (2), pp. 31-298, 1943.

ACCN: NNA.19900312.0151

Edwards A.L., TRUMP: A computer program for transient and steady state temperature distributions in multidimensional systems, National Technical Information Service, National Bureau of Standards, Springfield, Virginia, 1972.

ACCN: NNA.19910307.0131

Computer Models and their Development for the Unsaturated Zone Model at Yucca Mountain

- Hadley R.G., Theoretical treatment of evaporation front drying, *Int. J. Heat Mass Transfer*, 25(10), pp. 1511-1522, 1982.
ACCN: NNA.19890315.0016
- Hirschfelder J.O., C.F. Curtis, R.B. Bird, *Molecular theory of gases and liquids*, John Wiley and Sons, Inc., New York, 1954.
ACCN: NNA.19921202.0001
- International Formulation Committee, *A formulation of the thermodynamic properties of ordinary water substance*, IFC Secretariat, DÄsseldorf, Germany, 1967.
ACCN: NNA.19890918.0501
- Klinkenberg, L.J., The permeability of porous media to liquids and gases, in: *API Drilling and Production Practice*, pp. 200-213, 1941.
- Knudsen, M., *Die gesetze der molekularstroemung und der inneren reibungsstroemung der gase durch roehren, annalen der physik*, 28, pp. 75-131, 1909.
- Moridis, G., and K. Pruess, Flow and transport simulations using T2CG1, a package of conjugate gradient solvers for the TOUGH2 family of codes, Lawrence Berkeley National Laboratory Report LBL-36235, Lawrence Berkeley National Laboratory, Berkeley, California, 1995.
- Narasimhan, T.N., and P.A. Witherspoon, An integrated finite difference method for analyzing fluid flow in porous media, *Water Resources Research*, 12(1), pp. 57-64, 1976.
ACCN: NNA.19890522.0253
- O'Sullivan, M.J., G.S. Bodvarsson, K. Pruess, M.R. Blakely, Fluid and heat flow in gas-rich geothermal reservoirs, *Soc. Pet. Eng. J.*, 25, pp. 215-226, 1985.
ACCN: NNA.19910405.0017
- Peaceman, D.W., *Fundamentals of numerical reservoir simulation*, Elsevier, Amsterdam, 1977.
ACCN: NNA.19910405.0070
- Pritchett, J. W., M.H. Rice, T.D. Riney, Equation-of-state for water-carbon dioxide mixtures: implications for Baca Reservoir, Report DOE/ET/27163-8, Systems, Science and Software, La Jolla, California, February, 1981.
ACCN: NNA.19910405.0053
- Pruess, K., GMINC - A mesh generator for flow simulations in fractured reservoirs, Report LBL-15227, Lawrence Berkeley National Laboratory, Berkeley, California, 1983a.
ACCN: NNA.19910307.0134

Computer Models and their Development for the Unsaturated Zone Model at Yucca Mountain

- Pruess, K., Development of the general purpose simulator MULTKOM, Report LBL-15500, Annual Report for Earth Sciences Division - 1982, Lawrence Berkeley Laboratory, Berkeley, California, 1983b.
ACCN: NNA.19910307.0133
- Pruess, K., SHAFT, MULTKOM, TOUGH: A Set of numerical simulators for multiphase fluid and heat flow, Geothermia, Rev. Mex. Geoenergia, 4, pp. 185-202; also Report LBL-24430, Lawrence Berkeley National Laboratory, Berkeley, California, 1988.
ACCN: NNA.19910620.0128
- Pruess, K., T.N. Narasimhan, On fluid reserves and the production of superheated steam from fractured vapor-dominated thermal reservoirs, J. Geophys. Res., 87, (B11), pp. 9329-9339, 1982.
ACC: NNA.19900702.0038
- Pruess, K., T. N. Narasimhan, A practical method for modeling fluid and heat flow in fractured porous media, Soc. Pet. Eng. J., 25(1), p.14-26, 1985.
ACCN: NNA19890522.0235
- Pruess, K., Y. Tsang, Thermal modeling for a potential high-level nuclear waste repository at Yucca Mountain, Nevada, Report LBL-35381, Lawrence Berkeley National Laboratory, Berkeley, California, 1994.
ACCN: HQO.19940506.0005
- Pruess, K., TOUGH User's Guide, Nuclear Regulatory Commission, report NUREG/CR-4645, also Lawrence Berkeley Laboratory Report, LBL-20700, Berkeley, CA, 1987.
ACCN: NNA.19890315.0010
- Pruess, K., TOUGH2 - A general-purpose numerical simulator for multiphase fluid and heat flow, Lawrence Berkeley Laboratory Report, LBL-29400, Berkeley, CA, 1991.
ACCN: NNA.19940202.0088
- Pruess, K., A. Simmons, Y.S. Wu, G. Moridis, TOUGH2 software qualification, Lawrence Berkeley Laboratory Report, LBL-38383, Berkeley, CA, 1996.
- Pruess, K., J.S.Y. Wang, Y.W. Tsang, On thermohydrologic conditions near high-level nuclear wastes emplaced in partially saturated fractured tuff, part I. simulation studies with explicit consideration of fracture effects, Water Resources Res., 26(6), pp.1235-1248, 1990a.
- Pruess, K., J.S.Y. Wang, Y.W. Tsang, On the thermohydrologic conditions near high-level nuclear wastes emplaced in partially saturated fractured tuff, part 2. Effective continuum approximation, Water Resources Res., 26(6), pp.1249-1261, 1990b.
ACCN: NNA.19891026.0084

Computer Models and their Development for the Unsaturated Zone Model at Yucca Mountain

Rautman, C.A., Modeling spatial heterogeneity of thermal conductivity using a surrogate property, Proceedings of the Sixth Annual International Conference on High-Level Radioactive Waste Management, Las Vegas, NV, pp.83-84, 1995a.

ACCN: MOL.19950321.0080

Rautman, C.A., Preliminary geostatistical modeling of thermal conductivity for a cross section of Yucca Mountain, Nevada, Report, SAND 94-2283, WC-814, Sandia National Laboratory, Albuquerque, NM, 1995b.

DTN: SNSAND94228300.000 (Non-Q)

Sutton, F.M., and A. McNabb, Boiling Curves at Broadlands Field, New Zealand, N. Z. J. Sci. 20, pp. 333-337, 1977.

ACCN: NNA.19910405.0028

Warren, J.E., and P.J. Root, The behavior of naturally fractured reservoirs, Soc. Pet. Eng. J., pp. 245-255, Transactions, AIME, 228, 1963.

ACCN: NNA.19890522.0276

Wittwer, C., G. Chen, G.S. Bodvarsson, M. Chornack, A. Flint, L. Flint, E. Kwicklis, R. Spengler, Preliminary development of the LBL/USGS three-dimensional site-scale model of Yucca Mountain, Nevada, Report LBL-37356, UC-814, Lawrence Berkeley National Laboratory, Berkeley, CA, 1995.

Wu, Y.S., S. Finsterle, P. Fraser, C.F. Ahlers, and A. Simmons, Software qualification for ITOUGH2 and various equation-of-state (EOS) modules and auxiliary modules for TOUGH2 and ITOUGH2, Report LBL-xxxx, Lawrence Berkeley National Laboratory, Berkeley, CA, (draft).

GRID GENERATION AND ANALYSIS

C. Haukwa and G. Chen

August 1996

5.1 *Introduction*

Grid generation is an important part of development of a complex 3-dimensional 3-D model such as the UZ flow model for Yucca Mountain. The art of grid generation must achieve the proper balance between desired numerical accuracy in terms of gridblock size and computational time controlled by the total number of grid-blocks. Grids must also be adapted to the particular needs of the processes to be modeled because sharp gradients occur in different domains for flow processes. In this chapter we describe our three dimensional grid generation process, the development of two basic three dimensional grids to be used in UZ modeling studies and then finally describe the grid sensitivity studies.

5.2 *Development Of Mesh Generator For Complex Geometry*

Easy, accurate and efficient generation of a 2-D or 3-D numerical model is necessary for accurate modeling of subsurface fluid and heat transport. Major hydrogeologic features such as faults and layers with dips and pinchouts, have to be modeled explicitly. In some applications tunnels and boreholes also have to be explicitly modeled. Because models have to be frequently updated or evaluated inclusion of these features has to be easy and accurate.

The methods employed to develop the existing 3-D model are briefly discussed in chapter 5.1. A detailed report of these methods is presented by Wittwer et al (1992). Development of the numerical model using these methods typically will take 1-2 months. As an aid to mesh generation we are automating the process of generation of the 2-D and 3-D numerical models including faults with offsets. To achieve this, several programs that can be automatically linked are being developed. The main program is referred to as MGEN and employs the same geometrical methods used by the existing code "AMESH" developed by Fuller P. (see TOUGH2, Pruess K., 1990).

The code MGEN will generate a computational integral finite difference 2-D or 3-D mesh in a given domain. In the 2-D aerial plane, the Voronoi tessellation technique is used within the specified boundaries to create mesh of elements where the interfaces between neighbor elements are perpendicular bisectors of the line connecting the element centers. The interface distances are simply the medians of the line connecting the centers. In the vertical direction, the interfaces

are always treated as horizontal. In the lateral direction, the interface areas are always vertical, but direction of gravity vector takes into account the relative elevation of neighboring elements. This type of mesh is consistent with the computational requirements of the TOUGH2 numerical code simulator (Pruess K., 1990). The final output files 'eleme' and 'conne' will contain the element volumes and coordinates, and the connection information, suitable for direct input to the TOUGH2 numerical code. We are developing a user manual that will expand on different input options, data requirements and visualization features.

5.2.1 Input Data Structure

The primary type of data available for development of a 3-D model will vary. Hydrogeological data can be available in a variety of forms. For example, at Yucca Mountain these data are available as:

1. Surface and subsurface location of boreholes and tunnels. Location, dip, strike and offset of faults as well as the thickness of fault zones.
2. Description of each layer or horizon (hydrogeologic) unit using the aerial Cartesian system, for example, depth to horizon for each unit (isopach), dip of layers, thickness of layers, elevation of layers.
3. Surface maps of topography, alluvium deposits and hydrology.

Given a combination of the above data we require generation of a 3-D integral finite difference model (element and connections) suitable for input to a numerical simulation routine, e.g. TOUGH2. This model must accurately represent the conceptual model of the system. For TOUGH2 input, we require for all elements (including the fault and boundary elements), interface areas, interface distances and element volume at each xyz coordinate. We also require the same information for the embedded boreholes and tunnels.

Because of the variety of available base information, we will experiment with several data input formats for mesh generation. We have started with files that are similar to the existing input files for the mesh generation program "amesh". The xy points for the 2-D aerial grid and the isopachs that define the vertical hydrogeologic unit elevations are our primary starting points in the development of the 3-D grid. From the isopachs, the thickness of the individual sublayers are computed according to specified set of rules and an xyzt file ('x, y, z' coordinates and 't' thickness) for each 2-D nodal point developed. For nodal points that define elements along the trace of faults with offsets, only the z and t are computed by interpolation from isopachs on opposite sides of the fault. No two faults can be adjacent, i.e. faults must be separated by regular elements with specified xyz or xyt information. Faults without offsets are handled as regular elements with nodal points of elements aligned along the fault's trace.

In the input data specification, attention needs to be placed on the presentation of isopach data in order to accurately model the offsets across faults. In our mesh generation scheme it is necessary that isopachs be divided into blocks bounded by faults with offsets. However, in order to allow for accurate computation of layering near the faults with offsets and at model boundaries, a zone of overlap with neighboring blocks must be digitized in each block and near model boundaries.

Lateral boundaries are specified in an input file 'bound' that contains a sequence of xy data that describes a closed exterior boundary to all grid nodes. Convex and non-convex boundaries can be handled. If boundaries are faults with vertical offsets, then at least one set of regular (non-fault) elements beyond this boundary must be specified in order to obtain an interpolation of the offset. No special handling of top and bottom boundaries is required. These can be simply included as extra xyz or xyt points in the input file.

5.2.2 Code Description

The MGEN 3-D mesh generation program employs the Voronoi type mesh tessellation to generate the 2-D aerial mesh (block) first and then the 3-D mesh. A Voronoi block is a region of space that is closer to a grid point than to any other point in the same plane (Liuz et al, 1994). This method of mesh discretization fulfills the Integral Finite Difference method (IFDM) formulation of flow in porous media employed by TOUGH2. This scheme ensures that all interface connections in the plane are perpendicular to the flow directions.

When fully developed, this package of codes will incorporate both numerical grid and mesh visualization features. We are currently testing the 3-D numerical grid generation scheme that will incorporate a user interface for optional features. The current primary input file is the 'xyz' file developed from the two dimensional grid and the information on layering from the isopachs. This file can be generated from the corresponding xy data and the layer isopach data, by applying prescribed layer subdivision rules. The programs described below process this information to generate the TOUGH2 input files 'eleme' and 'conne' for domains that may include faults with offsets. This set of programs that now replace previously used mesh generation programs are named 'PARSE', 'BISECT', 'TOLER', 'MGEN', and 'DONE'.

1. 'PARSE'. Reads the input file of x and y's with layering information. An xy point without the z (layer thickness) information indicates a fault element from which the layering information will be computed from the elements on either side of it.
2. 'BISECT'. Reads an input file of boundary points (x and y's) one coordinate per line. There can be as many coordinates as are necessary to define the complex closed boundary using straight line segments. This program uses the boundary points and the interior points (nodes) to compute a Voronoi polygon around each node.

3. 'TOLER'. This deals with the minimum size of an interface, to avoid small connections in large grids. It eliminates small interfaces and merge the vertices at the ends of the eliminated interface.
4. 'MGEN'. Handles the layer geometry of the mesh.
5. 'DONE'. Computes the volumes and interface data and prints "eleme" and "conne", the final 3-D input files for the TOUGH2 program

By employing the above files in batch mode using prescribed files 'xyz' and 'bound' all the required element volume and connection information can be computed in one single step, eliminating the need for mechanical mesh fitting around the faults from individually generated section meshes. It also eliminates the need for creation of dummy elements and the verification of element connections. These program files will later be linked into a single mesh program MGEN so that all the required element volume and connection information can be computed in one single step using prescribed files 'xyz' and 'bound'. Generation of elements in this fashion will be extended to the explicit modeling of tunnels and boreholes in which transition from radial to rectangular geometry is desired and for local refinement within layers (for example near the repository drifts).

5.2.3 Mesh Validation

In order to validate the various mesh generation schemes, we will undertake studies to determine the sensitivity of numerical solutions to a given geometrical mesh generation scheme (for example the scheme for transition from radial to rectangular geometry during explicit modeling of tunnels and boreholes). Since the number of elements and the size contrast between elements in a given grid significantly affects the computational efficiency, every attempt is made to minimize the overall number of elements in the model and size contrast. We will investigate the sensitivity of modeling results to the number of numerical tunnel sectors and radial cells (rings around the tunnel) in order to determine the number sufficient to maintain consistency in moisture flow around the tunnel to available data. We will also investigate the number of transition layers required to reproduce the large contrast in saturation between the faults and the matrix, as well as various levels of mesh refinement.

5.2.4 Future Work

Mesh generation is based on the "xyzt" file as the primary input. As the number of faults with offsets increases, the number of zones required to generate these files becomes large and difficult to individually digitize. We are investigating the options of working directly from the given location of boreholes, tunnels, drifts, isopach maps, traces and offsets of faults to generate the 3-D mesh. We are also investigating options for generating cross-section and 3-D visualization of the mesh together with the TOUGH2 numerical output parameters, using "Earth Vision" (from Dynamic Graphics) which was used to the numerical simulation results (Chapter 7 and 8). These include options for 2-D

and 3-D visualization of the geometric mesh by layers, surfaces, elements, elevation, material properties, as well as inclusion of faults, tunnels, boreholes, view rotations, cut-out sections and data import from simulations. We will also look at options for mesh modifications or updates, e.g. addition or deletion of elements, faults, layers, tunnels, and boreholes as well as changes in boundary conditions.

5.2.5 Summary

We are developing the code MGEN to generate a computational Integral Finite Difference Method (IFDM) 2-D or 3-D mesh in a given domain. This code will allow for easy and accurate generation and modification of the 3-D Site Scale model of Yucca mountain. In the 2-D areal plane, the Voronoi tessellation technique will be used within the specified boundaries to create mesh of elements where the interfaces between neighbor elements are perpendicular bisectors of the line connecting the element centers. This type of mesh is consistent with the computational requirements of the TOUGH2 numerical code. The major requirement for this code is the ability to create a grid in which faults are explicitly modeled as discontinuities in which different layers (and material properties) interface across a vertical or inclined plane. Later we will extend this scheme to explicit modeling of tunnels and boreholes. Although our current primary input is the xyz or xyt data, we will experiment with several data input formats for generation of the grid, as well as alternative schemes for explicit modeling of faults, tunnels and boreholes. The different modules for data manipulation will be linked so that the mesh generation can be achieved in an automatic fashion. Numerical validation studies and analytical treatment will be used to determine accuracy of transition schemes particularly in explicit modeling of tunnels, boreholes and around locally refined areas.

5.3 *Development Of the 3-D Site Scale Model Grid Of Yucca Mountain*

We have developed new boundaries for the Site Scale model as an update to the 1992 3-D site scale model (Wittwer, et, al. 1992). The 1992 Site Scale model was based on fault map that provided explicit offsets on the Ghost Dance fault, the abandoned Wash and southern half of the Dune Wash fault. These were the only faults modeled with explicit offsets. The Solitario Canyon fault, the Bow Ridge fault and the proposed Yucca Wash fault were considered as model boundaries. Based on revised fault maps (see Chapter 2, Bandurraga, 1996), the observed shift in water level across the Solitario Canyon, the new infiltration and alluvium thickness maps, the observed pneumatic signals during the construction of the Exploratory Studies Facility (ESF) tunnel and the requirements for thermal loading studies we have developed revised boundaries for the Site Scale model. The new boundaries incorporate the high gradient potentiometric surface to the north of UZ-14 and explicitly includes the Solitario Canyon fault in the west and the Bow Ridge fault in the east, which

were treated as model boundaries in previous numerical studies. These new boundaries enclose most of the existing and planned hydrology boreholes and the boreholes with detailed hydrogeological data and lithology which are used as calibration points for formation properties (see Chapter 3, Bandurraga et al, 1996). Development of these 3-D models was based on new generalized geological layer isopachs over the extended region, from which the model vertical layers were computed. Details on model boundaries and hydrogeological layering are presented in Chapter 2 (Bandurraga et al, 1996).

In order to address the needs of specific studies, we have developed two 3-D grids of the site scale model at Yucca mountain, both based on the new geological model. The first grid, called the "FY96 UZ Model" grid, was used for the general unsaturated zone modeling and the study of the impact of thermal loading in the potential repository horizon (Chapters 8 and 13). The second grid called the "Gas effects" grid, was used to study the pneumatic impact of the ESF tunnel by Ahlers et al, (1996). The 3-D grids are designed to incorporate the spatial distribution of the main hydrogeological units, the effects of major structural features, and evaluate the sharp thermodynamic gradients at the boundaries between hydrogeological units.

The 3-D numerical grids were designed in two steps. The first step used all available surface information to create an horizontal two-dimensional grid. The second step integrated data from isopach maps of hydrogeological units to develop the vertical grid between the ground-surface and the water table. These models are an updates of the existing 3-D model developed by Wittwer, et al (1992). The development of these new models, like the old one, started with the definition of the grid block centers that defined a single 2-D horizontal grid to be used in all the 3-D vertical layer sections. After all the nodal points had been located, a numerical grid generator "amesh" was used to develop the horizontal 2-D grid. These 2-D horizontal grids and the sub-layering criteria were used to develop new 3-D Numerical grids of the unsaturated zone at Yucca mountain. The new grids were used for most of the numerical simulation studies of the unsaturated zone at Yucca mountain during FY 96.

The geological layering used is based on our new geological model (see Chapter 2, Bandurraga, 1996). Although most of the grid generation was carried out using the non-Q code "amesh", the methods employed follow documented and well established geometric principles and are similar to the mesh generation method used in the Q code TOUGH2.

5.3.1 2-D Areal extent of the FY96 UZ Model Grid

Figure 5.3.1, shows the 2-D aerial extension of the Site Scale "FY96 UZ Model" grid. One primary objective in the selection of the "FY96 UZ Model" grid boundaries was to minimize boundary effects due to thermal loading at the repository horizon and to investigate the influence of the major faults on the hydrological and thermal-hydrological response of the unsaturated zone (UZ), at ambient conditions and during thermal loading. The modeled area covers

nearly 40 km² and is bounded by Bow Ridge fault on the east, extends 1 km west of the Solitario Canyon, extends to the high potentiometric surface in the north, and is about 1 km south of the ESF south ramp. This grid considers thermal loading only in the "West Block Repository" area which is locally refined to an average size of 100x100m, and contains a maximum of 983 aerial grid block nodes in each layer. The 2-D FY96 UZ Model grid extends about 1 km west of the Solitario Canyon in order to explicitly model both the Solitario Canyon fault and its associated Iron Ridge fault branch to the south. Explicit modeling of the area west of the Solitario Canyon also allows for explicit specification of the 40 m rise in the water table west of this fault. This grid will be used to perform detailed studies related to repository thermal loading and for general Site-Scale model saturated and unsaturated zone modeling.

Figure 5.3.1

1996 Site Scale model, 2-D "FY96 UZ Model" grid, Circled numbers refer to model blocks used to define offsets across the major faults.

5.3.2 2-D Areal Extent of the Gas Effects Grid

Figure 5.3.2 shows the 2-D aerial extension of the Site Scale Gas Effects grid used by Ahlers et al (1996). The grid was designed primarily to allow for explicit modeling of observed pneumatic signals due to the ESF construction. The boundaries were therefore selected primarily to minimize boundary effects at the ESF or the observation boreholes (e.g., well ONC#1). This grid extends about 1 km west, north and south of the ESF drift and about 2 km east of the Bow Ridge fault. The modeled area covers nearly 32.5 km² and consists of a

maximum of 879 nodes in each layer. In this grid elements are aligned along the ESF drift to allow for prediction of ESF pneumatic effects. There is no local refinement or specification of a repository horizon in this model.

Figure 5.3.2
1996 Site Scale model, 2-D "Gas Effects" grid, Circled numbers refer to model blocks used to define offsets across the major faults.

5.3.3 Criteria for 2-D Grids

For both the FY96 UZ Model and the Gas Effects 2-D grids the following criteria were used for the choice of grid block centers.

1. Location of existing or planned boreholes are used as centers, subject to minimum spacing of 100 m between grid-blocks. Priority is given to boreholes that will be used for model calibration, like the UZ, SD, NRG, SRG, WT, and RF boreholes.
2. For the Gas Effects 2-D grid, blocks at an average spacing of 100 m were placed along the trace of the ESF and where any overlap occurred with existing or planned boreholes, the ESFESF block center was chosen.
3. For the FY96 UZ Model 2-D grid, locally refined grid block centers were placed at a spacing of 100m and aligned in the direction of the proposed repository drifts. Where an overlap occurred with the planned or existing boreholes or the trace of fault, the refined grid block center (repository block center) was used.

4. Elements were aligned along the trace of all the major faults to be explicitly modeled, ensuring that all elements along the faults have interfaces with only two neighboring fault elements, i.e. "back-to-back connection". In addition to this back-to-back connection, the elements are spaced such that fault elements in two neighboring faults are separated by at least a single row of non-fault blocks. This is necessary in order to uniquely compute the layer offsets across the faults.
5. Elements were also aligned based on the distribution (thickness) of the alluvial deposits, in order to accurately model the surface water infiltration rates, which is controlled by the alluvial distribution. A map of the alluvial distribution was obtained from EG&G (1994) which covers the extended model boundaries.

5.3.4 Development of the 3-D Numerical Grids

The 3-D grids were developed on the basis of the 2-D grids and the spatial distribution of main hydrogeological units. These units are the welded TCw and TSw (Tiva Canyon and Topopah Spring) and the non-welded PTn and CHn (Paintbrush and Calico Hills). A fixed number of vertical layers were chosen for each unit. This approach allowed for a lateral continuity of the layers. The new isopachs (Chapter 2, Bandurraga, 1996), provide explicit layer thicknesses for all the sublayers in the Paintbrush (five layers) and Calico Hills (ten layers). For the FY96 UZ Model 3-D grid, the TCw was divided into three sub layers in which the bottom layer was set at a maximum of 6.0 m and the remaining TCw subdivided equally into 2 two sub layers. The top of the model is represented by the top of the Tiva, i.e. ground surface minus the thickness of any alluvium. For the Gas Effects grid the alluvium thickness was explicitly modeled as a sub-layer on top of the Tiva in order provide for true surface pneumatic signal and any attenuation due to the alluvial layer (Ahlers, et al. 1996). The "CHn" is represented by four layers in the Calico Hills formation, two layers in each of the lower Prow Pass, Bullfrog, and Tram geologic layers. The TSw is subdivided into seven sub layers (Chapter 2, Bandurraga, 1996). These hydrogeological sub layers represent, as closely as possible, lithological variations within the main units.

For the FY96 UZ Model 3-D grid, because of the need to explicitly model the potential repository horizon at the proposed elevation, three additional sub-layers were included, mainly within TSw sub layer five corresponding to the middle nonlithophysal layer. The offsets along major fault zones (Solitario Canyon, Iron Ridge, Ghost Dance, Dune Wash, and the Bow Ridge faults) when explicitly modeled, are represented within the three-dimensional grid by horizontally connecting the sublayers on each side of the faults through a double number of gridblocks.

The amesh grid generator was adapted to generate the three-dimensional grid. In order to take into account the fault offsets within the columns of gridblocks located along the fault traces, the generation of the numerical grid was

performed in two steps by dealing first with all gridblocks except those including offsets, then taking care of gridblocks with offsets (the fault grid blocks). The grids for non-fault and fault sections were then combined to obtain the three-dimensional numerical grid for the whole site-scale model area. Two separate grid generation schemes were necessary because the number of vertical grid blocks in the fault areas is twice that of the surrounding grid blocks.

**5.3.4.1
Development of Grid-Blocks
with and without Fault
Offsets**

The only difficulty in generating the grid for all the grid-blocks outside the fault zones is to obtain the correct volumes and interfaces for the grid blocks adjacent to the faults. The modeled area was divided into six blocks. Each of those blocks was delimited by faults and/or model boundaries (Fig. 5.3.1 and 5.3.2). The offsets across the faults were defined by the elevation of the base of the Tiva in neighboring blocks. One block consists of all grid blocks located west of Solitario Canyon fault. The second block is pinched between Solitario Canyon faults and Iron Ridge faults. The third block is bounded by Solitario Canyon and Iron Ridge faults in the west, and the Ghost Dance fault in the east. The 4th zone is between the Ghost dance fault and the Dune Wash fault. The 5th zone between the Dune Wash and Bow Ridge faults. The last block is east of the Bow Ridge fault.

The FY96 UZ Model grid includes only the first five blocks, while the Gas Effects grid consists of only blocks 3-6. As a result, the mesh generator was run five times for the FY96 UZ Model grid and four times for the Gas Effects grid, to create sub-meshes of the grid. These sub-meshes were finally combined to provide the 3-D grid data (volumes, connections, interfaces) for the combined grid of each model.

The challenge in creating grid-blocks located along the fault traces is maintaining the sudden offset across the faults and the correct interfaces to adjacent blocks. To achieve this we divided each fault block element into two and adapted the mesh generator in order to connect them by their common interfaces to the adjacent grid-blocks. A schematic representation of this grid design is given in Figure 5.3.3.

Figure 5.3.3
Example of Grid Design in Fault Zones

5.3.4.2 The Combined 3-D Grid

Various programs have been written to choose, check, and recombine the files with connections and volumes from these two mesh generations as well as allocate material properties to each model element. For example, one of the programs reads all connection names within the output files and corrects them if they are not consistent with grid block names. Another program combines grid blocks and their connections from different output files of the mesh generator and is used for the addition of top and bottom layers of grid blocks over the entire model area to provide required boundary conditions such as saturation, temperature, and pressure during numerical simulations.

The final 3-D numerical grid is composed of two files "eleme" and "conne" which contain grid block location, volumes, and connections information suitable for a TOUGH2 input. The FY96 UZ Model grid consists of about 27,000 elements and 95,000 connections, while the Gas Effects grid consists of about 21,000 elements and 67,000 connections. These files are used as the basis for numerical simulations. Chosen cross-section can be extracted from these three-dimensional data sets for performing two-dimensional simulations. Fig 5.3.4 shows an east-west vertical cross-section from the new 3-D model of Yucca mountain. The model extends vertically to the water table at about 730 m. The hydrogeological layers and the vertical offsets at all major faults were explicitly developed by our grid generation process. The final model 3-D grid, shows good agreement with the geological model of Yucca Mountain (see Chapter 2, Bandurraga, et al., 1996).

Figure 5.3.4

East-West vertical cross-section through the 3-D model showing hydrogeological layering and offsets on the explicitly modeled faults.

5.3.5 Summary

We have developed 3-D grids within the extended boundaries of the Site Scale model of Yucca mountain. The first grid called the "FY96 UZ Model" grid has a locally refined repository area. This grid explicitly models the repository as a 6 m horizon at an average elevation of 1070 masl over the West Block area. It also explicitly models the Solitario Canyon, the Ghost Dance and the Dune Wash faults to assess their influences on hydrological and thermohydrological response of the UZ. This grid was used for general saturated and unsaturated zone modeling as well as for detailed studies related to Repository thermal loading. The second grid called the "Gas Effects" grid has locally refined nodes associated with the main ESF drift and was used for Pneumatic studies by Ahlers et al. (1996). This grid explicitly models the Ghost Dance, Dune Wash, and the Bow Ridge faults. In both grids the new hydrogeological isopachs developed from available borehole and surface data were used to generate the vertical layer thicknesses. These two 3-D models were the basis for most of the 1996 numerical studies of the UZ at Yucca mountain.

5.4 Grid Sensitivity Analysis in Numerical Modeling of the Unsaturated Zone

There are always concerns about numerical accuracy when coarse grids are used for large problems. We performed brief grid sensitivity studies with the Wittwer et al. (1992) model but have not explicitly presented them to the

project. Given the fact that questions arise often regarding grid orientation effects we decided to briefly summarize this work. Details of these studies are given in Bhogeswara (1994). The numerical simulations were carried out using the Q code TOUGH2.

In this work, grid refinement studies were conducted using two-dimensional vertical cross-sectional submodels extracted from the Wittwer et al. 1992 3-D numerical grid of the site-scale model of Yucca mountain. These two-dimensional cross-sectional submodels have non-uniform geometry, different hydrogeological units and variable rock properties. In these models the relationships between relative permeability and capillary pressure for the unsaturated rocks are predicted using Brooks and Corey (1966), and van Genuchten (1980) methods from the interpretation of experimentally measured capillary pressure versus saturation profiles using rock samples from Yucca Mountain. The equivalent continuum approximation described in Klavetter and Peters (1986), was used to integrate fracture flow to matrix flow for welded tuffs.

This study examined the effects of refining the grid vertically, horizontally, and in both directions, on the accuracy of our simulations. Since the problem of fluid movement through unsaturated zone with heterogeneous formation with stratified layers and fractures is highly nonlinear, the results from the grid refined in both directions are unlikely to be a direct sum of the results from the first two cases. The comparison among these three cases provides valuable information regarding the accuracy and computational efficiency of the original coarse grid. The following section describes design of three different fine grid models in more detail.

5.4.1 Design of Refined Grids

A fine grid model with horizontal refinement is designed by splitting each coarse gridblock into two new fine grid-blocks in the horizontal direction and replacing the coarse grid block center with two centers for the new fine grid-blocks. The fine grid model with horizontal refinement has twice as many cells and grid-blocks as coarse grid model. The geometric information, such as grid block volume, interface area, nodal distance and component of gravitational acceleration along nodal line, is recalculated using the locations of the new fine grid centers. This information is required as input for TOUGH2 simulator. The new fine grid-blocks are assigned same representative rock matrix properties and fracture properties as the corresponding original coarse grid-blocks. Fault zone properties for the fine grid block model is kept unchanged.

Similarly, the fine grid model with vertical refinement is designed by splitting each coarse grid block into two new fine grid-blocks in vertical direction, doubling the number of layers. The fine grid model with both vertical and horizontal refinement is designed by splitting each coarse grid block into two both vertically and horizontally. In all cases the rock properties for the new refined blocks correspond to the properties of the original coarse block.

The above approach for grid-blocks with regular geometry is modified for grid-blocks with irregular geometry with appropriate corrections for all three fine grid models. The original coarse grid contains 219 elements and 413 connections. The final refined grid models contain 438 elements and 827 connections for the fine grid block model with horizontal refinement, 427 elements and 829 connections for the fine grid block model with vertical refinement, and 854 elements and 1659 connections for the fine grid block model with both vertical and horizontal refinement.

5.4.2 Results of Numerical Simulations

Steady state simulations were performed using the TOUGH2 simulator at three spatially uniform infiltration rates of 10^{-1} , 10^{-2} and 10^{-3} mm/yr to obtain capillary pressure and saturation distributions on the original coarse grid model and also on the three different fine grid models described above. The results obtained using these four different numerical models are compared using the following approach:

a) Volume-Weighted Error Method: Saturation

In the volume-weighted method, liquid saturation is multiplied by pore volume to compare the volume of liquid saturation in the fine and coarse grids at steady state. We compared the results of the coarse grid to each of the fine grids. If the steady state solution of the coarse grid is as accurate as the fine grid solution, the error calculated remains close to zero.

The fine grid saturation, S_f is obtained by calculating the volume averaged saturation of the refined blocks incorporated within each original coarse block.

$$S_f = \frac{\sum_{i=1}^n V_{fi} S_{fi}}{\sum_{i=1}^n V_{fi}} \quad (5.4.1)$$

Where V_f is volume of the fine block, and n is the number of fine grid-blocks in each coarse gridblock

The volume-weighted error in saturation is given by absolute difference in saturation between the coarse grid and the average saturation for fine blocks in the coarse block.

$$dfsl = |S_c - S_f| \quad (5.4.2)$$

Where S_c is saturation in the coarse block

b) Volume-weighted Percentage Error Method: Saturation

Since the unsaturated zone at Yucca Mountain consists of highly heterogeneous formation with widely varying stratigraphy and faults, conditions vary from approximately zero to about full liquid saturation. The above described approach of calculating errors in saturation distributions may not be able give a relative estimate of error. To overcome this difficulty, the volume-weighted errors evaluated using the above approach were recalculated using the equation given below:

$$dfsl \% = \frac{dfsl}{S_f} \times 100 \quad (5.4.3)$$

This equation determines volume-weighted error as a percentage of liquid saturation for a given coarse gridblock. The volume-weighted percentage errors, as calculated in equation 5.4.3, are high in regions such as faults since the liquid saturation (denominator) is low.

c) Volume-Weighted Error Method:- Capillary Pressure

The volume-weighted effective saturation evaluated from the fine grid models is used to calculate capillary pressure from the characteristic curve of capillary pressure vs. saturation. The volume-weighted error in capillary pressure is calculated as the absolute difference between capillary pressure using the fine grid and coarse grid models as shown in the equation, 5.4.4 below:

$$dfpc = |P_{cf} - P_{cc}| \quad (5.4.4)$$

where P_{cc} is the coarse grid capillary pressure and P_{cf} is the fine grids capillary pressure.

d) Volume-Weighted Percentage Error Method:- Capillary Pressure

The difference in capillary pressure in the fine and coarse grid models is used to obtain the percentage error in capillary pressure for a given coarse gridblock using equation 5.4.5 shown below:

$$dfpc \% = \frac{dfpc}{P_{cf}} \times 100 \quad (5.4.5)$$

This section describes the results obtained from steady state capillary pressure and saturation distributions for the original coarse grid and also the three

different fine grid models. The results are presented in terms of actual distributions as well as in terms of volume-weighted error and volume-weighted percentage error for both saturation and capillary pressure. Though simulations and comparisons were performed for several infiltration rates, only selected results are shown in order to keep this report brief. We present below the results for an infiltration rate of 10^{-1} mm/yr.

5.4.2.1 Fine Grid with Horizontal Refinement

Using the fine grid with horizontal refinement, the volume-weighted percentage error is close to 1.2% for saturation and 5% for capillary pressure. Though there is some trend in grid block locations where errors in saturation and capillary pressure occur, the maximum percentage error in saturation does not necessarily correlate with that of capillary pressure due to the highly non-linear relationship between capillary pressure and saturation. For the most part, these errors can be considered negligible compared to the accuracy with which rock properties such as porosity, permeability and other hydrogeologic parameters are estimated. In general, the gridblock locations of errors in saturation and capillary pressure coincide with those where a maximum change in saturation (front) and capillary pressure are occurring compared to neighboring grid blocks i.e., at hydrogeological unit boundaries. These changes are better resolved on the fine grid model compared to the original coarse grid model. Since the characteristic nature of a fault zone makes it devoid of any liquid saturation, the percentage error in saturation at the faults are calculated to be larger because absolute gridblock saturations are smaller. For the grid with horizontal refinement, the maximum absolute difference in error is within 0.006 for saturation and 0.4 bar for capillary pressure.

5.4.2.2 Fine Grid Model with Vertical Refinement

The volume-weighted error and percentage errors in saturation and capillary pressure between the fine grid with vertical refinement and the original coarse grid show that these errors are predominant in areas where lateral flows in the TSw and/or faults exist. Lateral flow occurs in regions where a higher-permeability layer is underlain by a low-permeability layer, especially in the case of the TSw. In this unit, the top layers, in which lateral flow occurs, are two-orders of magnitude more permeable than bottom layers. Saturation fronts are resolved better using the fine grid with vertical refinement than with the original coarse grid. The maximum absolute magnitude of volume-weighted error in saturation is close to 0.026 in regions where lateral flow occurs. The volume-weighted percentage errors in saturation are close to 10% in grid blocks within the fault zone since low errors in this region result in large percentage errors because of small liquid saturations. The volume-weighted error in capillary pressure is close to 2.4 bars in regions where lateral flow is resolved better with the fine grid with vertical refinement. The volume-weighted percentage error in capillary pressure is close to 34% where lateral flow occurs, due to the highly non-linear and rapidly changing characteristic curves.

5.4.2.3 Fine Grid Model with Both Vertical and Horizontal Refinement

The volume-weighted error and percentage error in capillary pressure and saturation distributions for the fine grid model with both vertical and horizontal refinement resemble those of the fine grid model with vertical refinement in terms of the magnitudes and grid block locations of these errors. This may suggest that errors due to vertical refinement are more predominant than those due to horizontal refinement and also that accurate and computationally efficient results could be obtained by vertical refinement only.

The saturation fronts resulting from the fine grid fine grid model are better resolved compared to those of the original coarse grid. Figure 5.4.1 and 5.4.2 show the steady state distribution of saturation and capillary pressure using the original coarse grid and fine grid model at steady state. The volume-weighted percentage errors in saturation and capillary pressure are shown in Figures 5.4.3 and 5.4.4. These errors are predominant in the top layers of TSw and also in the fault zones for the same reasons explained in the case of fine grid model with vertical refinement. For the grid with both vertical and horizontal refinement, the volume weighted percentage error is close to 8% in saturation and 34% in capillary pressure. The absolute magnitude of volume-weighted error in saturation is close to 0.026 in saturation and 2.4 bar in capillary pressure. The grid blocks where these errors occur, are only a small percentage of the total number of grid blocks. A more accurate and computationally efficient modified coarse grid could be designed by refining only those layers of the coarse grid model where these errors occur. This type of study is very useful in redesigning the grid to obtain an accurate and efficient modified coarse grid model.

5.4.3 Summary

Grid refinement studies were performed on a vertical two-dimensional cross-sectional model of the 1992 three-dimensional site-scale numerical model of the unsaturated zone at Yucca Mountain. Various grid were used to evaluate the effect of vertical and horizontal refinement on the accuracy and computational efficiency of the 1992 numerical model. A "coarse" grid and three refined grids of the two-dimensional cross-sectional model were used: (1) A fine grid model with horizontal refinement, (2) a fine grid with vertical refinement, and (3) a fine grid model with both vertical and horizontal refinement. Steady state simulations were performed with the original coarse grid and also using three fine grid models to calculate saturation and capillary pressure distributions, using the numerical simulator TOUGH2. We used the volume-weighted error and percentage-error method to compare saturation and capillary pressure results obtained using these four numerical models. The errors in saturation and capillary pressure are within 10% except in limited regions. Larger errors occur in the dry fault zones and the highly saturated lateral flow zones where saturation fronts are resolved better by finer grids. Based on this study we conclude that an accurate and computationally efficient refined grid model can be obtained by refining the top few layers of TSw, in which errors in saturation and capillary pressure are large. In general, more accuracy is obtained with vertical refinement than with horizontal refinement. The results of this

study were used in the design of the new hydrogeological model isopachs and 3-D model grid sub-layers. For example the layers were increased from five to seven in the TSw (Chapter 2, Bandurraga, 1996).

Figure 5.4.1
Steady State Liquid Saturation distribution using the original coarse grid with an infiltration rate of 10-1 mm/year.

Figure 5.4.2
Steady State Capillary Pressure distribution using the original coarse grid with infiltration rate of 10-1 mm/year.

Figure 5.4.3

Volume-weighted percentage difference in Liquid Saturation between the coarse grid and the grid with vertical and horizontal refinement, for infiltration rate of 10-1 mm/year. Coarse grid configuration shown.

Figure 5.4.4

Volume-weighted percentage difference in Capillary Pressure between the coarse grid and the grid with vertical and horizontal refinement, for infiltration rate of 10-1 mm/year. Coarse grid configuration shown.

5.5 References

- Ahlers, C. F., C. Shan, C. Haukwa, A. J. B. Cohen, G. S. Bodvarsson, Calibration and prediction of pneumatic response at Yucca Mountain, Nevada, using the LBNL/USGS three-dimensional, site-scale model of the unsaturated zone, Yucca Mountain Project Milestone OB12M, Lawrence Berkeley National Laboratory, Berkeley, CA, 1996.
- Bhogeswara R., G. Chen, C. S. Wittwer, and G. S. Bodvarsson, Study of grid effects in numerical modeling of the unsaturated zone at Yucca Mountain, Lawrence Berkeley Laboratory Internal Report, Lawrence Berkeley Laboratory, Berkeley, CA, 1994.
- Brooks R. H., A.T. Corey, Properties of porous media affecting fluid flow, *Journal of Irrigation and Drainage Div.*, proceedings of the Am. Soc. Civ. Eng., 92, IR2, pp. 61-88, 1966.
ACCN: NNA.19870407.0356
- Klavetter E.A., R.R. Peters, Estimation of hydrologic properties of an unsaturated fractured rock mass, Soil, SAND84-2642, Sandia National Laboratories, 1986.
- Palagi, L. C., Generation and application of the Voronoi grid to model flow in heterogeneous reservoirs, Ph.D. thesis, Department of Petroleum Engineering, Stanford University, Palo Alto, CA, 1992.
- Pruess, K., TOUGH2 a general purpose numerical simulator for multiphase fluid and heat flow, Lawrence Berkeley Laboratory Report LBL-29400, Lawrence Berkeley Laboratory, Berkeley, CA, 1990.
ACCN: NNA.19940202.0088
- Van Genuchten. M., A closed form solution for predicting the properties the hydraulic conductivity of unsaturated soils, *Soil. Sci. Soc. Am. J.*, 44, pp. 892-898, 1980.
- Wittwer, C. S., G. S. Bodvarsson, M. P. Chornack, A. L. Flint, B. D. Lewis, R. W. Spengler, and C. A. Rautman, Design of a three-dimensional site scale-model for the unsaturated zone at Yucca Mountain, Nevada, *Proceedings of the Third International High Level Radioactive Waste Management Conference*, Las Vegas, NV, pp. 263-271, 1992.
ACCN: NNA.19930119.0139
DTN: GS911208312293.001 (Non-Q)

**INVESTIGATION OF CONCEPTUAL
AND NUMERICAL APPROACHES
FOR EVALUATING GAS, MOISTURE,
HEAT AND CHEMICAL TRANSPORT**

C. Doughty and G. S. Bodvarsson

August 1996

6.1 Introduction

The unsaturated zone (UZ) at the Yucca Mountain site is a complex system with a variety of important processes occurring at different scales. These processes include gravity and capillary driven moisture flow, gas convection and diffusion, transport of water and gas soluble chemicals and energy transport through conductive and convective processes. Superimposed on these processes are the flow continua that consist of fracture networks, major fault channels and rock matrix continuum, that gives rise to inter-continua processes such as fracture/matrix interaction, rock/fluid interaction and others. In addition, the potential repository will introduce a large thermal perturbation due to radioactive heat decay that will drastically alter most of the processes.

The UZ site-scale model must consider most if not all of the above processes. In order to do so efficiently a variety of numerical approaches must be considered. These include single-continuum, effective continuum, dual-continua, multiple-continua, explicit fracture discretization (e.g., for a fracture network with no matrix present), and explicit fracture and matrix discretization approaches. These different numerical methods vary greatly in complexity, ease of code convergence and consequently ease of computation. A proper numerical approach must be carefully chosen for each prevailing problem, depending upon the conceptual model that is envisioned for all relevant processes being considered.

The general approach in the UZ model development is to start by considering single processes using one- or two-dimensional models, obtain a satisfactory match with observed data and then proceed to consider additional processes or dimensions. It is expected that when one considers only a single process that primarily acts in a single continuum (either in the fracture network or solely in the rock matrix), that a single-continuum model will be appropriate. An example of this may be conductive heat transfer, if one believes that in the ambient state the convective component is small. When a different process is being considered, such as mountain-scale moisture flow, where at least two continua (fracture network and rock matrix) are present and active, one clearly must evoke an effective continuum approach, a dual-continua approach, or an explicit fracture discretization. The proper choice of these two numerical approaches may depend upon the boundary conditions (e.g. pulse or steady-state infiltration) and the time domain of interest (transient or steady state).

In this section we investigate the utility and appropriateness of the various numerical approaches for the processes of interest for the UZ flow model. A one-

dimensional column model, extracted from the three-dimensional UZ model is used, thus retaining some realism in the model with respect to geological layering and properties. A series of simulations is then performed using all of the above mentioned numerical approaches. After detailed comparisons of the results, recommendations are given for the selection of numerical approaches for various processes, including gas, moisture, heat and chemical transport.

6.2 QA Status of Data and Software used in this Chapter

Software

Several versions of the numerical simulator TOUGH2 are used in the present studies; all have been qualified. The qualification of the standard version (TOUGH2 Version 1.11), which uses the EOS3 equation of state module (water, air, and heat flow) is described in Pruess et al. (1996). The qualification of the liquid-flow only module, EOS9, and TOUGH2 with radionuclide transport is being conducted in conjunction with the present report (Wu et al., in press).

The inverse model ITOUGH2 was used to determine some of the material properties for the present studies. The qualification of ITOUGH2 is also being conducted in conjunction with the present report (Wu et al., in press)

Data

The material properties used in the TOUGH2 model for the present studies were obtained from three sources.

1. ITOUGH2 inversions of steady-state capillary pressure/liquid saturation data from qualified boreholes were used to determine fracture and matrix permeabilities and characteristic curve parameters (Chapter 3, Bandurraga et al.). Because both the data and ITOUGH2 are qualified, the resulting properties are qualified.
2. Porosity values do not affect steady-state calculations, so matrix and fracture porosities could not be determined by the ITOUGH2 inversion. Matrix porosities were taken from laboratory measurements on core samples (Flint, 1996). This data will be qualified.
3. Fracture porosities were taken from Ho (1995), who derived them from TSPA93 data (Wilson et al., 1994). This data is non-Q.

6.3 Numerical Formulations

Three classes of numerical formulations are used here to study fracture-matrix flow and transport: single-continuum models, effective continuum models, and dual-continua models. The numerical formulations are described

in the paragraphs below, summarized in Table 6.3.1, and illustrated schematically in Figure 6.3.1. Each formulation is used to study liquid and gas flow and heat and chemical transport for a column of the Yucca Mountain UZ site-scale model.

Explicit discretization of fractures (either as a stand-alone flow network or in conjunction with matrix interactions) is not considered practical for the site-scale model as a whole, in as much as there are estimated to be on the order of 10^9 fractures at Yucca Mountain. Therefore, it is not considered in the present studies. However, explicit fracture discretization may be very useful for studying particular features of interest, such as hydrologically important faults (See Chapter 10, Fairley, et al.).

Multiple-continua models consider the interaction of more than two hydrogeological components, such as matrix, multiple fracture sets, and faults. These models are also not considered in these studies because the available data set is not sufficient for extensive use of these models. A brief discussion of possible use of multi-continua models for the CI-36 issue and fast paths is given in Chapter 11, (Sonnenthal, et al.)

**6.3.1
Single-Continuum Models**

There are two types of single-continuum models: those which represent just the rock matrix, and those which represent just the fracture network. Neither single-continuum formulation is expected to accurately represent the true subsurface conditions at Yucca Mountain, wherein both fractures and matrix play an important role. However, these models may provide valuable insights into limiting behavior. For example, the fracture-network model represents the limit of the case in which fracture coatings or channelized fracture flow limit interaction with the rock matrix.

**6.3.2
Effective-Continuum Models**

In the effective continuum model (ECM) approach, each grid block includes a fracture and matrix component. In the traditional ECM, non-zero liquid saturation in the fracture does not occur until the matrix is fully saturated, which occurs at the so-called threshold saturation, defined as $S_{th} = V_m / (V_f + V_m)$, where V_f and V_m are the volumetric fractions of fracture and matrix, respectively. Special characteristic curves which embody matrix behavior for $S < S_{th}$ and fracture behavior for $S > S_{th}$ are constructed. In the generalized ECM described in Chapter 4 (Wu, et al.), the concept of threshold saturation is not invoked. Instead, liquid saturation is partitioned into the matrix and fracture in accordance with the principle of thermodynamic equilibrium, which requires capillary pressure in the matrix and fracture components of a grid block to be equal. Characteristic curves for the fracture and matrix components of the model are specified independently. Thus, in the generalized ECM formulation fracture flow occurs at all saturation, although small fracture flow is computed at low saturations. Note that the ECM only considers a single effective storativity for both the matrix and the fractures. Hence, full mixing is always assumed.

6.3.3 Dual-Continua Models

In the dual-continua approach, each grid block is subdivided into a fracture block and one or more matrix blocks (see Figure 6.3.1). If each fracture grid block is associated with only one matrix grid block, fracture-matrix flow must be approximated as quasi-steady. This treatment is the numerical equivalent of the Warren and Root (1963) formulation. On the other hand, if the rock matrix associated with a given fracture grid block is discretized into multiple grid blocks, transient fracture-matrix flow can be simulated. If global flow occurs only between fracture grid blocks, the model is known as a dual-porosity model, because fracture permeability alone controls large-scale flow, and the matrix just contributes an additional storage term. If global flow occurs within both fracture and matrix continua, the model is known as a dual-permeability model. TOUGH2 (Pruess, 1991, Appendix C) incorporates a mesh-making capability, known as the MINC (Multiple Interacting Continua) approach, to subdivide grid blocks into fracture and matrix components.

Figure 6.3.1
Schematic diagram of a one-dimensional column of grid blocks, modeled as a) ECM, b) dual-porosity with one matrix block per fracture block c) dual permeability with one matrix block per fracture block, and d) dual porosity with 3 matrix blocks per fracture block. Modified from Zimmerman et al. (1996).

There are two additional variations on the dual-continuum models. The first is conceptually equivalent to the multi-grid-block, dual-porosity method described above. However, grid blocks are only needed to represent the fracture network. Associated with each grid block is a source/sink term allowing fracture-matrix flow to be represented semi-analytically. Eliminating the grid blocks representing the rock matrix greatly improves the efficiency of the method. See Zimmerman et al. (1996) for a detailed description of this method, as well as a comparison of its use to a dual-porosity model and an ECM.

Investigation of Conceptual and Numerical Approaches for Evaluating Gas, Moisture, Heat and Chemical Transport

The second enhancement to a dual-continuum model is the use of a hysteretic capillary pressure/liquid saturation relationship for the matrix blocks. See Niemi and Bodvarsson (1991) for a detailed description of the hysteretic formulation. The hysteretic formulation may be used in conjunction with either dual-permeability or dual-porosity models, with either one or more matrix blocks. It will only produce different results from non-hysteretic models for problems which show non-monotonic moisture changes, such as occurs for a finite-duration pulse of high infiltration rate, or the drying and rewetting of matrix blocks as a result of thermal loading.

Table 6.3.1.
Types of numerical formulations for fracture-matrix flow.

Model	Subdivision of Grid Blocks	Type of Flow
Single Continuum Models		
matrix only	none	matrix-matrix
fracture only	none	fracture-fracture
Effective Continuum Model	none	fracture-fracture, matrix-matrix, (fracture-matrix flow is assumed to be instantaneous)
Dual Continua Models		
Dual-Porosity (Warren and Root)	1 fracture 1 matrix	fracture-fracture quasi-steady fracture-matrix
Dual Porosity (MINC)	1 fracture n matrix*	fracture-fracture, fracture-matrix
Dual-Permeability (Warren and Root)	1 fracture 1 matrix	fracture-fracture, matrix-matrix, quasi-steady fracture-matrix
Dual-Permeability (MINC)	1 fracture n matrix	fracture-fracture, matrix-matrix, fracture-matrix
Semi-Analytical Matrix Flow	none	fracture-fracture, fracture-matrix
Dual Permeability with Hysteresis (Warren and Root)	1 fracture 1 matrix	fracture-fracture, matrix-matrix, quasi-steady fracture-matrix
*Typically $3 \leq n \leq 10$, we have taken $n=5$.		

6.4 Conceptual Model Considered

6.4.1 Vertical Column Selected

A single column representing the location of well USW SD-7 was extracted from the three-dimensional site-scale model, as shown in Figure 6.4.1. It consists of 24 active grid blocks, 3 for the Tiva Canyon, 5 for the Paintbrush, 10 for the Topopah Springs, and 6 for the Calico Hills, and an overlying and underlying boundary block representing the atmosphere and the water table, respectively. This column was selected for various reasons. First, all of the data from SD-7 is qualified (Q-data); second, well SD-7 is a part of one of the most used East-West cross-sections in the UZ model, so that the results from this chapter can be cross-correlated to two-dimensional results in other sections; third, well SD-7 has a reasonably representative geological column with both vitric and zeolitic Calico Hills units present.

Figure 6.4.1
One-dimensional column extracted from the site-scale model of the unsaturated zone at Yucca Mountain, representative of conditions at well SD-7.

For each of the dual-continua models, the volume fraction of the fracture grid block is taken to be 0.001. The porosity of this block is chosen so that the product of porosity and volume fraction equals the true fracture porosity. For the MINC models, the remainder of the grid block (volume fraction 0.999) is subdivided into five matrix blocks, with volume fractions 0.004, 0.016, 0.064, 0.256, and 0.659, with the smallest volume adjacent to the fracture block. The characteristic fracture spacing is taken to be one meter, and fractures are assumed to form three orthogonal sets.

6.4.2
Properties and Boundary
Conditions

The material properties of the model were determined by matching moisture content/capillary pressure data using ITOUGH2, as described in Chapter 3 (Bandurraga, et al.). Properties were checked for consistency with pneumatic data (Ahlers, et al., 1996) and results of laboratory studies on core samples (Flint, 1996).

As discussed in Chapter 3 (Bandurraga et al) the available moisture tension and saturation data were matched using various infiltration rates. In the present study, we assumed a constant infiltration rate of 0.1 mm/yr and used the property values for all layers corresponding to the 0.1 mm/yr inversion. The assumed infiltration rate is the only ground surface boundary condition needed when only moisture flow, uncoupled from ambient temperature or gas flow, is considered. For cases involving coupled processes, constant temperature and gas pressure were also prescribed at the ground surface. The bottom boundary condition was located at the water table, and measured values of potential, temperature and other state variables were prescribed there.

The TOUGH2 inversion used the ECM formulation for all the units except the Paintbrush, which was modeled as a porous medium. The ECM formulation includes a complete set of hydrologic parameters for both fracture and matrix components of the model. For the single-continuum models, either the fracture or matrix properties were extracted from the ECM formulation. For the dual-continua models, the fracture properties of the ECM were assigned to the fracture grid blocks, and the matrix properties were assigned to the matrix grid blocks. As in the ECM, the Paintbrush was modeled as a porous medium. It is acknowledged that recent CL-36 data suggest throughgoing fracture flow in localized areas in the Paintbrush unit, in addition to flow down faults. The pneumatic data, however, suggests that those areas with sufficient fracture flow are few, and therefore, that the most reasonable representation of the Paintbrush is as a porous medium.

Porosities are not determined by the ITOUGH2 calibration to steady-state data. Matrix properties were taken from laboratory studies on core samples (Flint, 1996). The fracture porosity values of Ho (1995) were used for the base cases. Another set of parameters, from TSPA93 (Wilson et al., 1994), has also been used in sensitivity studies.

After initial studies of pneumatic response were complete, it was apparent that the smallest permeability in the Paintbrush unit (layer PTn23) was too small to allow enough of the barometric pressure variation signal to propagate into underlying layers. Therefore, the permeability of material PTn23 was increased by a factor of ten, which kept it within the range of permeabilities returned by various ITOUGH2 inversions for that layer. This increased permeability produced better agreement with the pneumatic data, and did not affect the steady-state moisture profile. It was used for all subsequent pneumatic, chemical transport, and thermal studies.

6.5 *Numerical Comparative Studies*

6.5.1

Steady-State Moisture Flow

Features of the Problem

For steady-state flow problems, the ECM approximation is expected to be valid since the pressure in the fractures and matrix are expected to be in near-equilibrium resulting in only minor inter-continua flow. Furthermore, because the flow equation is a diffusion equation, it tends to average over details, making the results relatively insensitive to the choice of numerical formulation. For liquid infiltration, gas may be treated as a passive spectator, using the EOS9 module of TOUGH2.

Procedure

We begin with a uniform liquid saturation of 0.70 throughout the model, and apply an infiltration rate of 0.1 mm/yr by adding a source term in the uppermost active (i.e., non-boundary) element of the model (the top Tiva Canyon element). The simulation is run to steady state. For the dual-permeability model, the source may be partitioned between the matrix and fractures or assigned entirely to the fractures. The former boundary condition is consistent with the ECM formulation, whereas the latter is required for the dual-porosity formulations. At steady state, the liquid saturation profile and the flow distribution between fractures and matrix are compared for the various numerical formulations.

Results

Figure 6.5.1 shows the steady-state liquid saturation profiles for fractures and matrix, obtained using the ECM. The ECM saturation is a weighted average of the fracture saturation and the matrix saturation, and because of the small fracture porosity (less than 0.001), it is nearly equal to the matrix saturation. For the Paintbrush unit ($1250 < z < 1270$ m), where there are no fractures, the fracture saturation is set equal to the matrix saturation.

Figure 6.5.1
Steady-state liquid saturation profile for 0.1 mm/yr infiltration, using the ECM.

Figure 6.5.2 shows the steady-state liquid saturation profiles obtained with the dual-permeability models using one or five grid blocks to represent the matrix (identified as the "1-k" and "5-k" models, respectively). For the 5-k model, both fracture and matrix saturation profiles are nearly identical to those of the ECM. For the 1-k model, the matrix saturations agree reasonably well with the 5-k model, but the fracture saturations are somewhat too high. This overprediction arises because during a wetting process, flow from fracture to matrix is underpredicted when only one grid block is used to represent the rock matrix.

Figure 6.5.2
Steady-state liquid saturation profile for 0.1 mm/yr infiltration, using the 1-5 and 5-k dual-permeability models.

Under steady flow conditions, the fracture and matrix flow at each depth must sum to equal the imposed infiltration rate. Figure 6.5.3 shows the steady-state fracture flow profiles for the 1-k and 5-k models. For an infiltration rate of 0.1 mm/yr, a substantial portion of the flow can occur through the matrix, therefore fracture flow is near zero over much of the profile. Only in the Tiva Canyon at 1340 m elevation and in the upper part of the Topopah Springs at 1170-1220 m elevation does fracture flow dominate. The inability of the 1-k model to produce a large enough fracture-to-matrix flow below these zones is manifested by the tails of overly high fracture flow.

Figure 6.5.3

Steady-state fracture flow profile for 0.1 mm/yr infiltration, using the dual-permeability models.

Because such a large portion of the flow can occur through the matrix for this low infiltration rate, the dual-porosity models, in which matrix-to-matrix flow is not considered, are expected to produce somewhat different results than do the ECM and dual-permeability models. Figure 6.5.4 shows the steady-state liquid saturation profiles obtained with the dual-porosity models. Identical results are obtained using the models with one or five grid blocks to represent the matrix (identified as the "1-p" and "5-p" models, respectively). Furthermore, a single-continuum fracture-only model (the model is matrix-only for the Paintbrush) also produces identical results for the fracture saturation profile. This consistency of results among different models is expected, as each model treats the fractures identically, and the fracture flow alone must balance the imposed infiltration rate.

Figure 6.5.4
Steady-state liquid saturation profile for 0.1 mm/yr infiltration, using the 1-p and 5-p dual-porosity models.

The liquid saturations obtained with the dual-porosity and fracture-only models are higher in the fractures than they are the ECM or dual-continuum models, because without a matrix flow component, the fractures must carry more flow. Hence they require greater relative permeability, which is achieved through higher liquid saturation. Because capillary equilibrium is reached between matrix and fractures for steady-state flow, the matrix saturation is also higher for the dual-porosity models. For higher infiltration rates, a greater component of the flow will occur in the fractures, decreasing the differences between the dual-permeability and dual-porosity models.

Summary

All the numerical formulations give similar results for steady-state liquid saturation profiles. The means by which liquid flow occurs (fracture versus matrix flow) depends strongly on whether or not matrix to matrix flow is allowed, but such a choice belongs more in the realm of conceptual modeling rather than numerical modeling. When matrix-to-matrix flow is desired, because of its efficiency and robustness, the ECM is judged to be the preferred choice for modeling steady-state liquid flow.

6.5.2 Transient Moisture flow

Features of the Problem

Gas may be treated as a passive spectator, using the EOS9 module of TOUGH2. For transient flow problems, the ECM may or may not provide a good representation of fracture and matrix flow, depending on the time scales for fracture-fracture flow and for fracture-matrix flow. An estimate of the time required for a matrix block to equilibrate with a fracture block during an imbibition or drying process is given by:

$$t_{fm} = \frac{4\mu_l \alpha_m \phi_m}{k_m} (V_m / A_m)^2 \quad (6.5.1)$$

where μ_l is the viscosity of the pore water, and $(\alpha_m, \phi_m, V_m, A_m, \text{ and } k_m)$ are the van Genuchten parameter, porosity, volume, surface area, and permeability of a typical matrix block (Zimmerman et al., 1995). The quotient V_m / A_m describes a characteristic length scale for matrix blocks, which we take to be one meter.

In contrast, the time required for a liquid pulse with flow rate q to propagate through a fracture block of thickness Δz , in the absence of matrix interactions, can be approximated by

$$t_{ff} = \frac{\Delta z \phi_f S_l}{\min(K_{sat}, q)} = \frac{\Delta z \phi_f S_l}{\min\left(\frac{k_f \rho_l g}{\mu_l}, q\right)} \quad (6.5.2)$$

where ϕ_f is fracture porosity, S_l is liquid saturation, and K_{sat} is fracture saturated hydraulic conductivity ($K_{sat} = k_f \rho_l g / \mu_l$, where k_f is fracture permeability, ρ_l is the density of water, and g is gravitational acceleration). When $K_{sat} < q$ ponding occurs and $S_l = 1$. When $k_{sat} > q$, S_l will be less than one, and will depend on the details of the matrix and fracture characteristic curves. As a simple approximation we use $S_l = 1$, with the caveat that the actual transit time will be faster for $S_l < 1$ (e.g., for Figure 6.5.2: $0.1 \leq S_l \leq 0.2$).

The ECM is expected to work well when $t_{ff} \gg t_{fm}$, that is, when there is ample time for fracture-matrix flow to occur before global fracture-fracture flow across a grid block is complete. Table 6.5.1 shows these times for selected elements of the one-column model, for several flow rates. As flow rate increases, the ECM formulation is seen to be appropriate for fewer elements. We have found that in practice, Equations (6.5.1) and (6.5.2) provide conservative bounds, and the ECM may work well beyond the range they suggest.

Investigation of Conceptual and Numerical Approaches for Evaluating Gas, Moisture, Heat and Chemical Transport

Procedure

We begin with the equilibrated moisture distribution for 0.1 mm/yr infiltration, and apply a one-week pulse of large infiltration rate to the uppermost active element in the column, then return to an infiltration rate of 0.1 mm/yr. Saturation changes at various locations are used to track the wetting front.

Table 6.5.1. Fracture-fracture and fracture-matrix characteristic times*				
Material	0.1 mm/yr t_{ff} (yr)	10 mm/yr t_{ff} (yr)	Ponding t_{ff} (day)	t_{fm} (yr)
TCw	125	1.2	3.E-03	0.4
PTn	12180	121.8	18.7	2.E-02
TSw	73	0.7	2.E-03	1.7
CH Vitric	46	0.5	7.E-03	0.1
CH Zeolitic	13	0.1	2.E-02	0.6
PP Vitric	62	0.6	0.2	0.2
PP Zeolitic	36	0.4	4.E-02	3.8
*calculated from Equations (6.5.1) and (6.5.2), using properties and element thicknesses from the site-scale model and $V_m/A_m = 1\text{ m}$, $\mu_l = 10^{-3}$ Pa sec, $\rho_l = 10^3$ kg/m ³ , and $g = 10$ m/s ² , assuming $S_l = 1$.				

The maximum liquid flow that can pass through an element under a unit hydraulic gradient (gravity flow) is given by the maximum saturated hydraulic conductivity of that element, which is generally the fracture conductivity, although it could also be the matrix conductivity for sparse fracturing. This conductivity is denoted the flow-controlling conductivity. For the Paintbrush unit, in which fractures are not considered, the flow-controlling conductivity is simply the saturated hydraulic conductivity of the porous medium. The one-week pulse infiltration rate is chosen to be much greater than the minimum flow-controlling conductivity in the column, so that as soon as the pulse reaches the level of the flow-controlling conductivity, ponding occurs. The pressure then increases above this level, and in the top element in the column where the source is located, some of the flow is diverted to the overlying element, which is held at atmospheric pressure. Thereafter, the model is equivalent to one in which a ponded boundary condition is applied at the top of the model. At early times, before ponding occurs, the imposed infiltration rate underestimates the flow into the model compared to a ponded boundary condition. For the column being studied, the minimum flow-controlling conductivity occurs in the Paintbrush unit.

Results

Table 6.5.2 summarizes the times at which liquid saturation changes by a few percent of its maximum change, an arbitrary measure chosen to approximate the arrival of the wetting front, at the lowermost element in the Topopah Springs and just above the water table (the lowermost element in the Calico Hills). The different methods produce large differences in arrival time, which

Investigation of Conceptual and Numerical Approaches for Evaluating Gas, Moisture, Heat and Chemical Transport

can be explained by examining the liquid saturation as a function of time for various depths in the model, these data are shown in Figures 6.5.5 through 6.5.11. Note that in these figures, initial conditions are the saturation profiles resulting from 0.1 mm/yr infiltration, which differ slightly from model to model. Time is plotted on a log scale. The high-infiltration-rate pulse ends at one week (0.02 years), after which time infiltration at 0.1 mm/yr resumes.

Table 6.5.2. Times at which saturation increases at the bottom of the Topopah Springs and at the bottom of the Calico Hills for a one-week high-infiltration-rate pulse		
Model	Bottom of Topopah Springs (years)	Bottom of Calico Hills (years)
ECM	800	7000
Dual permeability, one matrix block (1-k)	5	6000
Dual permeability, five matrix blocks (5-k)	1200	8000
Dual porosity, one matrix block (1-p)	1.5	1000
Dual porosity, five matrix blocks (5-p)	60	3000
Fracture Only	0.7	0.7
Dual permeability, five matrix blocks (5-k), limited fracture-matrix area	3-1200	60-8000
*On a Pentium-100 personal computer		

Figure 6.5.5 shows saturation transients for the ECM. Recall that for this model, ECM saturation is very close to matrix saturation, but that under the assumption of equilibrium between matrix and fractures, the times at which saturation changes at a given depth will be the same for the matrix and the fractures. A saturation increase at the bottom of the Tiva Canyon begins quickly, even before the one-week pulse has ended. The pulse takes much longer to reach the bottom of the Topopah Springs (about 800 years) and Calico Hills (about 7000 years).

Figure 6.5.5

Liquid saturation as a function of time at the bottom of each hydrological unit and in the upper portion of the Topopah, for a one-week pulse of high infiltration, using the ECM.

Figures 6.5.6 and 6.5.7 show saturation transients for the 1-k model and 5-k model, respectively. The arrival times for the 5-k model agree reasonably well with those of the ECM, however, the arrival time at the bottom of the Topopah Springs for the 1-k model is markedly shorter (5 years compared to about 1000 years.) The two saturation transients shown for the Topopah Springs display a double-humped shape for the dual-permeability models which is absent in the ECM. The first arrival represents fracture flow, while the second represents matrix flow. Because the ECM treats fracture and matrix flow as occurring concurrently, these sequential arrivals cannot be obtained with the ECM. Furthermore, the 1-k model predicts a much larger fracture-flow arrival than does the 5-k model, an indication of the underprediction of fracture-to-matrix flow that has already been noted for the 1-k model in conjunction with uniform infiltration.

Figure 6.5.6
Liquid saturation in the fractures as a function of time at the bottom of each hydrogeologic unit and in the upper portion of the Topopah, for a one-week pulse of high infiltration, using the 1-k model.

Figure 6.5.7
Liquid saturation in the fractures as a function of time at the bottom of each hydrogeologic unit and in the upper portion of the Topopah, for a one-week pulse of high infiltration, using the 5-k model.

Figures 6.5.8 and 6.5.9 show saturation transients for the 1-p model and 5-p model, respectively. Because all downward flow occurs through the fractures, the saturation transients do not show the complex structure associated with the

dual-permeability models. However, just as for the dual-permeability models, the 1-p model predicts much shorter arrival times than does the 5-p model, again suggesting an underprediction of fracture-to-matrix flow with the 1-p model.

Figure 6.5.8
Liquid saturation in the fractures as a function of time at the bottom of each hydrogeologic unit and in the upper portion of the Topopah, for a one-week pulse of high infiltration, using the 1-p model.

Figure 6.5.9
Liquid saturation in the fractures as a function of time at the bottom of each hydrogeologic unit and in the upper portion of the Topopah, for a one-week pulse of high infiltration, using the 5-p model.

Figure 6.5.10 shows saturation transients for the fracture-only model. Because there are no fractures in the Paintbrush, the model is matrix-only there. Arrival times for all depths below the Paintbrush are similar for this case, about

Investigation of Conceptual and Numerical Approaches for Evaluating Gas, Moisture, Heat and Chemical Transport

0.7 years, which is much earlier than for the previous cases, illustrating the overall importance of fracture-matrix interactions.

Figure 6.5.10

Liquid saturation in the fractures as a function of time at the bottom of each hydrogeologic unit and in the upper portion of the Topopah, for a one-week pulse of high infiltration, using the fracture-only model.

Figure 6.5.11 shows saturation transients obtained with the 5-k model by sequentially decreasing the area available for fracture-matrix flow, for the locations within and at the bottom of the Topopah Springs hydrogeologic unit. For these calculations, it was necessary to assign the entire infiltration to the fracture grid block, rather than partitioning it between the fracture and the matrix, as is generally done for dual-permeability calculations, otherwise ponding occurred in the matrix of the Tiva Canyon and pressures increased unrealistically. It is clear from the growth of the fracture arrival that as the fracture and matrix become more isolated from each other, preferential flow through the fractures increases. Furthermore, the effect of the preferential fracture flow grows with depth, so that by the bottom of the Topopah Springs, it shortens arrival time by nearly three orders of magnitude.

Figure 6.5.11

Liquid saturation in the fractures as a function of time for a one-week pulse of high infiltration, using the 5-k model, and a range of areas for fracture-matrix interaction. As area decreases, liquid saturation changes in the fractures occur earlier.

The above studies can be compared to a recent study by Zimmerman et al. (1996), which examined the response to ponded boundary conditions for an ECM, a dual-porosity model with 10 matrix blocks per fracture grid block, and a dual-porosity model using the semi-analytical approach for fracture-matrix flow. This study used a single-vertical column in which all fractures had a permeability of 10 d, and matrix properties were taken from an older version of the UZ site-scale model (Wittwer, et al., 1995). Fractures were included in the Paintbrush as well as in all the welded units. As shown in Table 6.5.1, for ponded boundary conditions, the fracture-matrix equilibration time is long compared to the time for fracture-to-fracture flow, suggesting that the ECM will be inadequate. This was definitely found to be the case in Zimmerman et al.'s study. The inclusion of high-permeability fractures in the Paintbrush caused the overall groundwater transit time from surface to the water table to be extremely short, on the order of one day, as calculated by the dual-porosity models (the discretized matrix blocks and semi-analytical method agreed closely). However, the ECM predicted changes in liquid saturation had reached only about 10 m below the ground surface after this time. The much shorter transit time to the water table obtained by Zimmerman et al. (1 day) compared to the present studies (0.7 years or longer) is consistent with the much larger flow-controlling conductivity used for their study, which is about a factor of 150 larger than the one used here.

Conclusions

The choice of numerical formulation makes a large difference for transient flow problems in which the time to reach fracture-matrix equilibrium is long compared to the time for fracture-to-fracture flow. Under these conditions, which typically arise from ponded boundary conditions, or other short-duration pulses of high infiltration rate, the ECM may greatly underpredict fracture flow. However, for smaller perturbations to the system, or for cases in which low-permeability layers limit flow in underlying fractured media (such a Paintbrush without high-permeability fractures), the ECM may be adequate. Among the dual-continua models, serious numerical errors may arise when only one grid block is used to represent the matrix. See Chapter 10 (Fairley et al.) for related calculations of pulse flow, using an explicit discretization of a fault zone.

6.5.3 Transient Gas Flow

Features of the Problem

As for liquid flow, gas flow is governed by a diffusion equation, which tends to average over heterogeneities. However, gas behaves very differently than liquid because of the great difference in gas and liquid properties. For example, gravity is a dominant effect for liquid flow, but practically negligible for gas flow due to the low density of gas. A characteristic time required for a gas pressure signal to propagate a distance d through a single continuum is estimated by the diffusion time:

$$t_g = \frac{d^2}{4 \left(\frac{k_g}{\mu_g \phi \beta_g} \right)} = \frac{d^2}{4 \left(\frac{k}{\mu_g \phi \beta_g} \right)} \quad (6.5.3)$$

where k_g is the permeability available to gas flow, (approximated as $S_g k$, with S_g gas saturation and k permeability), μ_g is the viscosity of gas, ϕ_g is the pore space available to gas flow ($\phi_g = S_g \phi$, where ϕ is total pore space), and β_g is gas compressibility ($\beta_g = 1/P_g$ for an ideal gas). The value of t_g is shown in Table 6.5.3 for properties representative of the hydrogeologic units that appear in the one-column model being studied. A distance of $d=1$ m has been used. These times are all very short relative to the characteristic times for fracture-fracture or fracture-matrix liquid flow, given in Table 6.5.1. Therefore, the pneumatic response to barometric pressure variations can be studied with an immobile liquid phase, making this a single-phase flow problem. The EOS3 module of TOUGH2 is used for the calculations.

Procedure

We begin with the steady-state moisture distributions arising from 0.1 mm/yr infiltration rate. Then, the characteristic curves are modified to make the liquid phase immobile and assign the gas phase a relative permeability equal to gas saturation. This may be simply accomplished with the van Genuchten (1980) characteristic curves by increasing residual liquid saturation to a

Investigation of Conceptual and Numerical Approaches for Evaluating Gas, Moisture, Heat and Chemical Transport

Table 6.5.3.
Gas-flow diffusion time *

Material	t_g (day)
TCw	1.3
PTn	3.E-03
TSw	2.1
CH Vitric	8.E-03
CH Zeolitic	16.5
PP Vitric	3.E-02
PP Zeolitic	8.8
Fracture	5.E-07
*calculated from Equation (6.5.3) using properties from the site-scale model and $d=1m$, $\mu_g=1.8 \times 10^{-5}$ Pa sec, $\beta_g=10^{-5}Pa^{-1}$	

value of 0.9999, which is greater than any saturation value present, and modifying the code to set gas relative permeability $k_{rg}=S_g$ instead of the usual value of $k_{rg}=1-k_{rl}$. We then transform from the EOS9 state variable (S_l) to the EOS3 state variables (P_g and S_l), and run a gravity equilibration to get the gas-static pressure profile. Finally, we apply a five-week sequence of time-dependent atmospheric pressure boundary conditions, by assigning a time-dependent pressure to the atmospheric element overlying the column. These atmospheric pressures are typical of values obtained at Yucca Mountain (Ahlers, et al., 1995; Rousseau, et al., 1996; Ahlers, et al., 1996), but do not necessarily represent any single location. The resulting pressure transients are observed at four depths in the column, corresponding to the bottom element of the Tiva Canyon, the Paintbrush, the Topopah Springs, and the Calico Hills hydrologic units.

Results

As in other pneumatic response studies (Ahlers, et al., 1995; Rousseau, et al., 1996; Ahlers, et al., 1996), no noticeable attenuation of the barometric pressure variation occurs in the Tiva Canyon, but a strong attenuation occurs over the Paintbrush. The ECM and both dual-permeability models give the same results (Figure 6.5.12) suggesting that gas flow from fracture to matrix occurs very quickly, on the time scale of the barometric pressure variations. This finding is consistent with the diffusion times shown in Table 6.5.3, for fracture spacings on the order of one meter.

The dual-porosity models have higher liquid saturation, resulting in decreased values of both permeability to gas k_g , and porosity available to gas, ϕ_g . However, as shown by Ahlers et al. (1996), for a fractured/matrix system, the fracture permeability and matrix plus fracture porosities should be used to calculate the diffusivity. Therefore, the increase in liquid saturation results in a larger diffusivity, and hence slightly less attenuation of the pneumatic signal

Investigation of Conceptual and Numerical Approaches for Evaluating Gas, Moisture, Heat and Chemical Transport

with depth (Figure 6.5.13). These results show that the total gas-filled porosity (matrix plus fracture) must be used in the analysis of the pneumatic data.

The fracture-only model has the same liquid saturation as the dual-porosity models, but shows even less attenuation of the signal over the Paintbrush, because of the smaller storativity due to the lack of matrix porosity in the underlying Topopah Springs (Figure 6.5.14).

Figure 6.5.12 Pneumatic response for the ECM and dual-permeability models at the bottom of the various hydrogeologic units.

Figure 6.5.13 Pneumatic response for the dual-porosity models at the bottom of the various hydrogeologic units.

Figure 6.5.14
Pneumatic response for the fracture-only model at the bottom of the various hydrogeologic units.

Conclusions

All the numerical formulations give similar results for the transient gas pressure response to barometric pressure variations. As for steady liquid flow, the only difference is whether or not matrix-to-matrix flow is allowed. Because of its efficiency, the ECM is judged to be the preferred choice for modeling transient gas-phase flow. It should be noted that we have recently completed a new EOS module for TOUGH2 (EOS1G), where only gas flow is computed analogous to the Richard's equation module for only water flow (EOS9). This module has been qualified and is described in Chapter 4 (Wu et al); it results in much improvement in computational efficiency for gas-flow calculations.

6.5.4 Tracer Transport

Features of the Problem

In contrast to the steady flow problem, for transient transport within a steady-state flow field, the equilibrium assumption for fracture-matrix interactions is not expected to be adequate. In addition, the transport equation has an advective term, which does not average over details, but tends to emphasize them, making the results much more sensitive to the choice of numerical formulation. The EOS3 module of TOUGH2 with an added tracer transport capability is used for the calculations.

Procedure

After difficulties in obtaining results using some of the numerical formulations with the original one-column grid, a simpler geological model was chosen for these tracer studies, in which there is no vertical variation in fracture or

matrix properties. Properties were chosen to be representative of a Topopah Spring layer in which a significant portion of the flow occurs through the fracture. Although the complexities arising from layering of the site-scale-model are missing, the basic fracture-matrix interaction is present, making this a meaningful case to study. After a steady state flow is established for an infiltration rate of 0.1 mm/yr, a conservative tracer is applied as a mass source in the uppermost grid block of the column. The tracer breakthrough as a function of time is examined at various depths, in both the fractures and the matrix.

Results

Tracer breakthrough curves at various locations in the column are shown in Figures 6.5.15 through 6.5.20, and summarized in Table 6.5.4. The ECM grossly overpredicts the tracer arrival time at the bottom of the Topopah Springs and at the bottom of the Calico Hills, compared to the other models. Results for the dual-continua models show that fracture and matrix tracer breakthrough times differ by orders of magnitude, which the ECM cannot accommodate. Results for the two dual-permeability models agree closely for early times (Figures 6.5.16 and 6.5.17), but begin to diverge slightly for later times when matrix transport, which the 5-k model calculates more accurately, becomes significant. The dual-porosity and fracture-only models (Figures 6.5.18 and 6.5.19) predict much earlier tracer breakthroughs than do the dual-permeability models, because the tracer source is applied solely to the fracture rather than partially to the fracture and partially to the matrix. The 1-p and 5-p models produce nearly identical results; they differ from the fracture-only model during the final portion of the breakthrough curve, when an elongated tail suggests diffusion caused by matrix interactions.

The tracer breakthrough times are quite sensitive to the partitioning of the source, as shown in Figure 6.5.20, which shows a 1-k run with the source assigned solely to the fracture. The early part of the fracture breakthrough curves agree closely with those for the dual porosity and fracture-only models, in which the source is also assigned solely to the fracture. Only at late times, when the matrix concentrations in the model begin to rise appreciably, do the fracture breakthrough curves differ. This suggests that for the parameters chosen, flow is dominated by advection, and diffusion plays only a minor role.

Figure 6.5.15

Tracer concentration as a function of time at depths corresponding to the bottom of the TCw, PTn, TSw, and CHn, for a model with no vertical variation in properties, for an infiltration rate of 0.1 mm/yr, using the ECM.

Figure 6.5.16

Tracer concentration as a function of time for a model with no vertical variation in properties for an infiltration rate of 0.1 mm/yr, using the 1-k model.

Figure 6.5.17

Tracer concentration as a function of time for a model with no vertical variation in properties for an infiltration rate of 0.1 mm/yr, using the 5-k model.

Figure 6.5.18

Tracer concentration as a function of time at depths corresponding to the bottom of the TCw, PTn, TSw, and CHn, for a model with no vertical variation in properties, for an infiltration rate of 0.1 mm/yr, using the 1-p and the 5-p models.

Figure 6.5.19

Tracer concentration as a function of time at depths corresponding to the bottom of the TCw, PTn, TSw, and CHn, for a model with no vertical variation in properties, for an infiltration rate of 0.1 mm/yr, using the fracture-only model.

Figure 6.5.20

Tracer concentration as a function of time for a model with no vertical variation in properties for an infiltration rate of 0.1 mm/yr, using the 1-k model with the source in the fracture only.

Table 6.5.4. Times at which tracer appears at depths corresponding to the bottom of the Topopah Springs and the bottom of the Calico Hills, for uniform infiltration of 0.1 mm/yr.		
Model	Bottom of Topopah Springs (years)	Bottom of Calico Hills (years)
ECM	10^5	$2 \cdot 10^5$
Dual permeability, one matrix block (1-k)	500	500
Dual permeability, five matrix blocks (5-k)	500	500
Dual porosity, one matrix block (1-p)	50	100
Dual porosity, five matrix blocks (5-p)	50	100
Fracture Only	50	100
Dual permeability, one matrix block (1-k) source in fracture only	50	100
*On a Pentium-100 personal computer		

Conclusions

These results must be viewed as preliminary, because they used such a simplified geological model, in which no vertical variation in properties occurs. We know from previous studies that vertical variability has a large effect on any model predictions. In particular, the back-and-forth flow between matrix and fractures that must occur for fracture flow such as shown in Figure 6.5.3 will provide greatly enhanced opportunities for spreading of tracer between fracture and matrix continua. Future work will incorporate tracer transport studies into the one-column model extracted from the site-scale model. However, it is safe to say that the choice of numerical formulation for fracture-matrix interaction has a dominant effect on tracer transport.

6.5.5 Thermal loading

Features of the Problem

This is a much more complicated problem than the previous ones, due to the presence of both multiphase flow and heat transport, along with strong phase-change effects. Heat transport occurs via both conductive and convective (heat-pipe) mechanisms. The interplay between fluid flow and heat trans-

port which occurs in a heat pipe, coupled with the very different time-scales for fluid flow in the fractures and the matrix, makes it likely that the ECM approximation will not be adequate. The EOS3 module of TOUGH2 is used for the calculations.

Procedure

We start with an equilibrated moisture distribution for 0.1 mm/yr infiltration obtained with EOS9, which is converted to EOS3 format. In order to obtain steady initial temperature and pressure profiles, we apply constant temperature boundary conditions at the water table (32° C) and the atmosphere (17° C), and a constant pressure boundary condition at the water table (0.94 bars). The volume of the atmospheric element is reduced, enabling pressure there to vary, while a large heat capacity keeps temperature constant. A mass source equivalent to 0.1 mm/yr of infiltration is applied, and the model is allowed to run to steady state. For the thermal loading calculation we apply a time-dependent thermal source equivalent to an initial thermal load of 83 kW/acre at the repository level. The 0.1 mm/yr infiltration rate continues. Transient temperature, liquid saturation, and fluxes are then observed at various locations.

Preliminary calculations using the original spatial discretization taken from the site-scale model, shown in Figure 6.4.1, suggested that spatial discretization around the repository (10 m thick elements above and below a 6 m thick repository) was not fine enough to represent the heat transfer correctly. Therefore, each of the 10 m thick elements over and underlying the repository element was subdivided into three elements, with thicknesses 1, 3, and 6 m, with the finest element adjacent to the repository.

Calculations were conducted for the ECM, the dual-permeability model with one matrix grid block per fracture grid block (the 1-k model), and the dual-porosity model with one matrix grid block per fracture grid block (the 1-p model). Calculations for the dual-continua models with multiple matrix grid blocks per fracture grid block will be conducted in the future.

Results

Figures 6.5.21 through 6.5.23 show transient temperatures, liquid saturations, and fluxes at various levels of the one-dimensional column, obtained using the ECM. At the repository level, the temperature (Figure 6.5.21) increases steadily to the boiling temperature of about 97° C, at which time liquid saturation begins to decrease (Figure 6.5.22). As drying continues, temperature remains at the boiling temperature, and a counter-current liquid and vapor flow develops (Figure 6.5.23), both above and below the repository.

Investigation of Conceptual and Numerical Approaches for Evaluating Gas, Moisture, Heat and Chemical Transport

Figure 6.5.21 Temperature as a function of time at the bottom of each hydrogeologic unit and at the repository, for an initial thermal load of 83 kW/acre and a 0.1 mm/yr infiltration rate, obtained with the ECM.

Figure 6.5.22 Liquid saturation as a function of time at the bottom of each hydrogeologic unit and at the repository, for an initial thermal load of 83 kW/acre and a 0.1 mm/yr infiltration rate, obtained with the ECM.

Figure 6.5.23

Mass flow rate as a function of time above and below the repository, for an initial thermal load of 83 kW/acre and a 0.1 mm/yr infiltration rate, obtained with the ECM. (Positive mass flow rate is downward.)

At ten years, the magnitudes of liquid flow above and below the repository are about 0.07 and 0.02 kg/s, respectively. Assuming a latent heat of 2.3 MJ/kg, the combined convective heat transfer away from the repository is 0.2 MJ/s, compared to the total heat load to 0.3 MJ/s, illustrating that heat transfer away from the repository is largely occurring via a heat pipe mechanism (thermal conduction accounts for the remaining heat transfer). The heat pipe above the repository carries the majority of the energy because gravity and capillary forces combine to drive liquid back toward the repository, whereas below the repository, capillarity must overcome gravity. For both heat pipes, the gas (steam) flow away from the repository is greater than liquid flow toward it, explaining the net drying that takes place during this period (see Figure 6.5.22).

When the repository level is completely dried out ($S_l=0$ at about 30 years), heat transfer must occur conductively, so temperatures increase. As the thermal load decreases with time, repository temperatures decrease as well, and when they drop to the boiling temperature, liquid saturation begins to increase and a smaller heat pipe develops, at about 800 years.

Overall, the results for the dual-continua models are similar to those of the ECM, with a combination of conductive and convective heat flows transporting

heat away from the repository, but important differences exist. Figures 6.5.24 through 6.5.27 show transient temperatures, liquid saturations, and fluxes obtained using the dual-permeability 1-k model. At any given depth, temperature is the same in the matrix and fractures. The early-time temperature transient (before dryout begins) is identical to the ECM. This is as expected for conduction-dominated heat flow. After temperature reaches the boiling temperature (about 8 years in both models), liquid saturation begins to decrease, but unlike in the ECM, in the 1-k model, complete dryout happens earlier in the fractures (about 30 years) than in the matrix (about 150 years). Therefore, the heat pipe continues to operate longer in the 1-k model, until the matrix dries out.

Figure 6.5.24
Temperature as a function of time at the bottom of each hydrogeologic unit and at the repository, for an initial thermal load of 83 kW/acre and a 0.1 mm/yr infiltration rate, obtained with the 1-k model.

Investigation of Conceptual and Numerical Approaches for Evaluating Gas, Moisture, Heat and Chemical Transport

Figure 6.5.25 Liquid saturation as a function of time at the bottom of each hydrogeologic unit and at the repository, for an initial thermal load of 83 kW/acre and a 0.1 mm/yr infiltration rate, obtained with the 1-k model.

Figure 6.5.26 Mass flow rate as a function of time above the repository, for an initial thermal load of 83 kW/acre and a 0.1 mm/yr infiltration rate, obtained with the 1-k model. (Positive mass flow rate is downward.)

Figure 6.5.27

Mass flow rate as a function of time below the repository, for an initial thermal load of 83 kW/acre and a 0.1 mm/yr infiltration rate, obtained with the 1-k model. (Positive mass flow rate is downward.)

Figures 6.5.28 through 6.5.30 show transient temperatures, liquid saturations, and fluxes obtained using the dual-porosity 1-p model. As in the dual-permeability model, at any given depth, temperature is the same in the matrix and fractures. The dual-porosity model (1-p) is similar to the dual-permeability model, except that because the dual-porosity model is wetter in both matrix and fractures to start with (see Section 6.5.1), the dryout period is longer, and the heat-pipe a relatively more important form of heat transfer.

Investigation of Conceptual and Numerical Approaches for Evaluating Gas, Moisture, Heat and Chemical Transport

Figure 6.5.28 Temperature as a function of time at the bottom of each hydrogeologic unit and at the repository, for an initial thermal load of 83 kW/acre and a 0.1 mm/yr infiltration rate, obtained with the 1-p model.

Figure 6.5.29 Liquid saturation as a function of time at the bottom of each hydrogeologic unit and at the repository, for an initial thermal load of 83 kW/acre and a 0.1 mm/yr infiltration rate, obtained with the 1-p model.

Figure 6.5.30

Mass flow rate as a function of time above and below the repository, for an initial thermal load of 83 kW/acre and a 0.1 mm/yr infiltration rate, obtained with the 1-p model. (Positive mass flow rate is downward.)

Conclusions

The general features of the heat transport and fluid flow for the thermal loading problem are similar for the ECM and dual-continua models. However, the ECM cannot resolve the separate time scales for fluid flow within the fracture network and the rock matrix, and because of the importance of convective heat flow, this has a major effect on the temperature and moisture conditions at the repository horizon.

6.6 Summary and Conclusions

A series of calculations were performed using a variety of numerical formulations to represent a fractured medium in which both fracture network and rock matrix play important roles in controlling flow and transport. The problems considered and the recommended numerical method are summarized in Table 6.6.1. Consideration of explicit fracture discretization has not been included in the present study, but it is admitted that there may be important processes for which it is required.

Steady-state calculations use qualified data, and conclusions drawn from them are therefore qualified. Transient calculations use both to-be-qualified

Investigation of Conceptual and Numerical Approaches for Evaluating Gas, Moisture, Heat and Chemical Transport

data (matrix porosities) and non-Q data (fracture porosities), therefore all conclusions regarding transient calculations including tracer transport and thermal loading are non-Q. We plan to repeat the suite of calculations included in this report using qualified fracture porosity data, thereby enabling qualified conclusions to be drawn. While the conclusions drawn from the results presented in this report are expected to be generally applicable to the UZ site-scale model, detailed results are likely to change for different material properties, spatial discretizations, etc.

Table 6.6.1.
Summary of problems considered.

Problem	Recommended Numerical Formulation
Steady-state moisture flow	ECM
Transient moisture flow	Dual-continua
Transient gas flow	ECM
Tracer transport	Dual-continua
Thermal Loading	Dual-continua

6.6.1 Comparison of Physical- Process Representation

In general, the ECM works well for steady-state problems because under steady-state conditions the equilibrium assumed between matrix and fracture components is true. The ECM also works well for transient gas flow problems because gas flow between matrix and fractures occurs quickly compared to the time-scale of gas pressure variations. However, for transient moisture flow problems, the ECM can grossly underestimate the transit time of a liquid pulse through a fracture network, because it assumes that each fracture element equilibrates with all the adjoining rock matrix, which can greatly slow down the pulse. Furthermore, the one matrix grid block per fracture grid block formulations introduced spurious fracture flows, suggesting that multiple matrix grid blocks are necessary to properly quantify transient fracture and matrix flow. Liquid pulse flow occurs not only for large infiltration events from the ground surface, but also during the convective heat transport mechanism known as a heat-pipe associated with thermal loading. Convective heat transport itself may be greatly underestimated by the ECM in comparison to the dual-continua models as well. Similarly, tracer transport is greatly underestimated by the ECM.

6.6.2 Comparison of Numerical Performance

Of all the numerical models considered, the single-continuum models run the most efficiently, but for most problems relevant to the UZ model of Yucca Mountain are inadequate to properly represent the physical processes of interest. The ECM requires no more numerical discretization than does a single-continuum model, and the overhead associated with the ECM formulation (enforcing equilibrium between fracture and matrix components) is very low, making the ECM nearly as efficient as a single-continuum model. Furthermore, we have found the ECM to be very robust for all the problems considered, with

little if any degradation in performance as material properties and boundary conditions are varied.

There is significantly more complexity associated with the dual-continua models than with the ECM because of the addition of a second time scale for fracture-matrix flow, which may be very different than the time scale for fracture-fracture flow. Therefore, the dual-continua models can be much more sensitive to the details of the problem, such as contrasts in material properties between adjacent layers, or strongly forcing boundary conditions. Under optimal conditions, the dual-continua models with one matrix grid block per fracture grid block (the 1-k and 1-p models) are expected to run about twice as slowly as the ECM, and the dual-continua models with five matrix grid blocks per fracture grid block (the 5-k and 5-p models) are expected to run about six times as slowly as the ECM, because computation time is roughly proportional to the number of grid blocks. An additional slow down may occur when smaller grid blocks are used, because smaller time steps may be required to achieve convergence. However, depending on the physics of the problem, dual-continua calculation times can vary greatly.

For the transient gas flow problems described in Section 6.5.3, in which the liquid phase is considered to be immobile, the computation times were roughly proportional to the number of grid blocks (more precisely, proportional to the number of connections, making the 5-p model faster than the 5-k model), and all numerical formulations were equally robust, with no trouble encountered for any of the calculations.

In contrast, the numerical performance of all the dual-continua models was at least somewhat sensitive to material properties and boundary conditions when liquid flow occurred. One feature of the present study that poses particular difficulties for the dual-permeability models is the great variation in fracture and matrix permeabilities throughout the column. Thus, flow does not simply occur in either the fractures or the matrix, but as illustrated in Figure 6.5.3, often must pass back and forth between them. We have found that varying a single material property (the van Genuchten α parameter for a fracture) for one layer caused a factor of five improvement in calculation time for a steady-state infiltration simulation using the 5-k model. By decreasing α_f , the fracture became wetter and the adjoining matrix drier, increasing fracture relative permeability, and therefore increasing the fraction of fracture flow. This result is consistent with the finding that we generally achieve better numerical performance for higher infiltration rates, in which more flow occurs in the fractures over most of the model.

6.7 References

- Ahlers, C. F., T. M. Bandurraga, G. S. Bodvarsson, G. Chen, S. Finsterle, and Yu-Shu Wu, Summary of model calibration and sensitivity studies using the LBNL/USGS three-dimensional unsaturated zone site scale model, Yucca Mountain Project Milestone 3GLM107M, Lawrence Berkeley Laboratory, Berkeley, CA, 1995.
DTN: LB092995312293.001 (Non-Q)
ACCN: MOL.19960208.0091-0097
- Ahlers, C.F., C. Shan, C. Haukwa, A.J.B. Cohen, and G.S. Bodvarsson, Calibration and prediction of pneumatic response at Yucca Mountain, Nevada using the LBNL/USGS three-dimensional site-scale model of the unsaturated zone, Yucca Mountain Project Milestone OB12M, Lawrence Berkeley Laboratory, Berkeley, CA, 1996.
- Flint, L., Matrix properties of hydrogeologic units at Yucca Mountain, Nevada, U.S. Geological Survey report, U.S. Geological Survey, Denver, CO, 1996 (draft).
DTN GS 950308312231.002 Q
- Ho, C., Assessing alternative conceptual models of fracture flow, in Proceedings of the TOUGH WorkshOp '95, K. Pruess editor, Lawrence Berkeley Laboratory Report LBL-37200, Lawrence Berkeley Laboratory, Berkeley, CA, 1995.
- Niemi, A. and G.S. Bodvarsson, Preliminary capillary hysteresis simulations for fractured rocks - model development and results of simulations, Lawrence Berkeley Laboratory Report LBL-23593, Lawrence Berkeley Laboratory, Berkeley, CA, 1991.
- Pruess, K., TOUGH2 - A general-purpose numerical simulator for multiphase fluid and heat flow, Lawrence Berkeley Laboratory Report LBL-29400, Lawrence Berkeley Laboratory, Berkeley, CA, 1991.
ACCN: NNA.19940202.088
- Pruess, K., A. Simmons, Y.S. Wu, and G.J. Moridis, TOUGH2 software qualification report, Lawrence Berkeley Laboratory Report LBL-38383, UC-814, Lawrence Berkeley Laboratory, Berkeley, CA, 1996.
- Rousseau, J.P., Data transmittal of pneumatic pressure records from 10/24/1994 through 3/31/96 for boreholes UE-25 UZ#4, UE-25 UZ#5, USW NRG-6, USW NRG-7a, USW SD-12, USW UZ-7a, from Yucca Mountain, Nevada, U.S. Geological Survey preliminary data, U.S. Geological Survey, Denver, CO, 1996. DTN: GS950508312232.004 Q
DTN: GS960308312232.001 Q
- van Genuchten, M.Th., A closed-form equation for predicting the hydraulic conductivity of unsaturated soils, Soil Sci. Soc. Amer. J., 44, pp. 892-898, 1980.

Investigation of Conceptual and Numerical Approaches for Evaluating Gas, Moisture, Heat and Chemical Transport

Warren, J.E. and P.J. Root, The behavior of naturally fractured reservoirs, Soc. Pet. Eng. J., 228, pp. 245-255, 1963.
ACCN# NNA 19890522.0276

Wilson, M.L., J.H. Gauthier, R.W. Barnard, G.E. Barr, H.A. Dockery, E. Dunn, R.R. Eaton, D.C. Guerin, N. Lu, M.J. Martinez, R. Nilson, C.A. Rautman, T.H. Robey, B. Ross, E.E. Ryder, A.R. Schenker, S.A. Shannon, L.H. Skinner, W.G. Halsey, J.D. Gansemer, L.C. Lewis, A.D. Lamont, I.R. Triay, A. Meijer, and D.E. Morris, Total-system performance assessment for Yucca Mountain - SNL second iteration (TSPA-1993), Sandia National Laboratories Report SAND93-2675, UC-814, Sandia National Laboratories, Albuquerque, NM, 1994.
ACCN: NNA19940112.0123

Wittwer C., G. Chen, G.S. Bodvarsson, M. Chornack, A. Flint, L. Flint, E. Kwicklis, and R. Spengler, Preliminary development of the LBL/USGS three-dimensional site-scale model of Yucca Mountain, Nevada, Lawrence Berkeley National Laboratory Report LBL-37356, UC-814, Lawrence Berkeley National Laboratory, Berkeley, CA, 1995.

Wu, Y.S., S. Finsterle, P. Fraser, C.F. Ahlers, and A. Simmons, Software qualification for ITOUGH2 and various equation-of-state (EOS) modules and auxiliary modules for TOUGH2 and ITOUGH2, Report LBL-xxxx, Lawrence Berkeley National Laboratory, Berkeley, CA, (draft).

Zimmerman, R.W., T. Hadgu, and G.S. Bodvarsson, Transient dual-porosity simulations of unsaturated flow in fractured rocks, Lawrence Berkeley Laboratory Report LBL-36807, Lawrence Berkeley Laboratory, Berkeley, CA, 1995.
DTN GS950208312281.001 (Non-Q)

Zimmerman, R.W., T. Hadgu, and G.S. Bodvarsson, Coupling of the semi-analytical simulation procedure to the LBNL/USGS site-scale model of the unsaturated zone at the Yucca Mountain, Yucca Mountain Project Milestone 2GLF101M, Lawrence Berkeley Laboratory, Berkeley, CA, 1996.

PERCHED WATER ANALYSIS

Y.S. Wu, G. Chen, and G.S. Bodvarsson

August 1996

7.1 Introduction

One of the primary objectives of developing the three-dimensional site-scale unsaturated zone model is to evaluate the movement of water, gas and heat in the unsaturated zone of Yucca Mountain and to study the effects of these dynamic processes on the performance of the potential high-level nuclear waste repository. The unsaturated zone at Yucca Mountain is about 500 to 700 m thick, depending on the local topography. The potential repository is located at the highly fractured, Topopah Spring welded unit, which is about 225 m above the water table. As a part of the site characterization efforts, a systematic drilling program has been carried out over the years to study the geological, hydrological, and geothermal conditions in the unsaturated and saturated zones of the mountain. During drilling, perched water zones were encountered in a number of boreholes (Burger and Scofield, 1994; OCRWM, 1995a; and Rousseau et al., (1996). The presence of perched water bodies within the mountain has important implications for the travel times and flow paths of water through the unsaturated zone, and may pose a potential problem for the construction, operation, and performance of the repository. Thus, it is necessary to incorporate observed perched water data into the site-scale model and calibrate the model against these data to better represent the hydrogeological conditions of the mountain.

Perched water can be defined as a saturated zone not directly connected to the static water table (Freeze and Cherry, 1979). There must exist two conditions for perched water to occur in unsaturated zones. The first condition is that water saturation should be sufficiently high to initiate substantial flow, and the second one is that the water pressure within the perched water volume has built up to values higher than static atmospheric gas pressure that would be expected at the same elevation. Under those conditions, water will flow freely into a borehole when the perched water body is intersected by boreholes. Perched water may accumulate where large hydraulic conductivity differences exist between adjacent formation units, when water migrating downward through a more permeable rock reaches a less permeable rock and has limited paths to continue downward flow. It could occur in a permeable layer overlying a relatively impermeable layer, or in a well-connected fractured unit overlying a locally unfractured or poorly connected fractured unit. It has been found that the relative fracture density and fracture permeability have a strong influence on the accumulation of perched water (Burger and Scofield, 1994). Perched water could also exist against a fault along a dipping horizontal plane if the fault acts as a capillary barrier to downdip water flow.

For the studies presented in this report, we selected five boreholes with perched water because of the relative large amount of information available for these boreholes (Burger and Scofield, 1994; Czarnecki, 1995; and Rousseau et al., 1996). The perched water bodies in most of these boreholes were detected in the layer of the bottom at the Topopah Spring unit (TSw) and the top of the Calico Hills unit.

The presence of perched water bodies in the vicinity of the potential repository at Yucca Mountain has many implications; perched water may provide useful information or insight on the moisture movement, flow pathways, and surface infiltration history within the mountain. The first implication of the existence of a perched water body is that percolation flux does not go straight down through the unsaturated zone to the water table. The water has been diverted laterally by a perched water body and then has flowed through a fault zone or a higher permeable channel to reach the water table. As a result, a very nonuniform water table recharge rate is expected. Also, the existence of perched water zones along the base of the TSw unit implies that water may not flow across the underlying zeolitic unit, and we may not get the benefits of retardation factors of these zeolites for slowing down radionuclide transport.

In this study, we have conducted a series of three-dimensional modeling simulations to investigate the perched water occurrences at the Yucca Mountain site using the TOUGH2 code (Pruess, 1991) and the available observation data of perched water occurrences from 5 boreholes, USW UZ-1, UZ-14, NRG-7a, SD-7, and SD-9. We have developed three models which incorporate the observed perched water data. One model is based on a sub-site-scale model, which contains boreholes UZ-1/14, SD-9 and NRG-7a. The 3-D submodel has a local refined (R-z) grid connected to UZ-14 for pumping test analysis. The other two use the entire current site-scale model grid. In these simulations, the generalized ECM method has been used to account for fracture and matrix interactions. An areally distributed infiltration map (Hevesi and Flint, 1995) is employed to describe the soil surface infiltration condition, and TOUGH2 simulations are run to steady-state. A second, newer infiltration map (Flint et al., 1996) is being used in the perched water studies. The predicted perched water locations and volume are compared with observed data, and reasonable agreement has been obtained.

7.2 *QA Status of Data and Software*

All the saturation and water potential data from Boreholes UZ-1/14, SD-9, NRG-7a and SD-7 are "QA" data, and have been used in this study for rock property estimation and perched water calibrations. Among the perched water zones identified in four boreholes (UZ-1, UZ-14, SD-9 and NRG-7a), the data regarding perched water at UZ-1 were collected prior to implementation of the approved USGS-YMP quality assurance program, and these data are "non-Q"

Perched Water Analysis

(Rousseau et al., 1996). However, observations of depths to and relation to lithostratigraphy for perched water at UZ-14, SD-9 and NRG-7a are fully qualified at USGS.

The TOUGH2 code has been used as a primary computer tool in this simulation study, and it has been qualified for the YMP site characterization studies (Pruess et al., 1996). We also use two additional modules, the ECM module of TOUGH2 and the ITOUGH2 code, an inverse model of TOUGH2 as discussed in Chapter 3, and they are both qualified for use in the YMP (Finsterle et al., 1996).

7.3 Perched Water Data

Several perched water occurrences in the unsaturated zone of Yucca Mountain were reported by Burger and Scofield (1994). Perched water occurred just below a zone of fractured rock in boreholes, UZ-1, USW UZ-14, NRG-7/7a, and SD-9. The perched water information for borehole USW SD-7 was obtained from Czarnecki (1995) and Soeder (1995). In addition to the perched water information, the measured saturation and water potential profiles available for all the selected boreholes were also used to compare with the simulation results presented in Chapter 8 (Wu et al., 1996).

The locations of the five selected boreholes are shown in Figure 7.3.1.1. The coordinates and related information for these boreholes are listed in Table 7.3.1. Detailed descriptions of the boreholes and of the perched water are presented below.

Table 7.3.1 Borehole location and perched water occurrence						
Boreholes	Nevada Coordinates ¹		Surface Elevation ²	Total Depth ²	Top of Perched Zone	
	North (m)	East (m)	(masl)	(m)	Elevation (masl)	Depth (m)
UZ-1	-235085	170755	1349	387	967	381
UZ-14	-235095	170731	1349	597	966	383
NRG-7a	-234355	171598	1282	461	821	458-461
SD-7	-231328	171066	1359 ⁵	632	880	480 ⁵

Perched Water Analysis

Table 7.3.1 (cont.) Borehole location and perched water occurrence						
	Nevada Coordinates ¹		Surface Elevation ²	Total Depth ²	Perched Level ⁴	
SD-9	-234086	171242	1302	678	889	413

¹ Yucca Mountain Site Characterization Project, Site Atlas (1994).
² Yucca Mountain Project Borehole Lithostratigraphy Compilation (Preliminary Draft, 1995).
³ Yucca Mountain Site Characterization Project, Site Atlas Supplement (1993).
⁴ Burger and Scofield (1994).
⁵ Czarnecki (1995) and Soeder (1995).

7.3.1 Borehole Perched Water Data

Figure 7.3.1.1

Locations of boreholes with perched water occurrence and a plan view of the site-scale model domain, showing model boundary, computational grid, major incorporated faults, and the Exploratory Study Facility (ESF).

Perched Water Analysis

7.3.1.1 Boreholes UZ-1/14

Borehole USW UZ-1 is located in Drill Hole Wash, north of the potential repository area (Figure 7.3.1.1), at the surface elevation of 1,349 m above sea level. The possible perched water zone was detected in or just below the base of the Topopah Spring Tuff of the Paintbrush Group at a depth of 387 m. Borehole UZ-14 is located less than 30 m from UZ-1 in Drill Hole Wash at an elevation of 1,349 m. The borehole was drilled to a total depth of 387 m, and perched water was encountered at a depth of about 383 m, near the basal vitrophyre of the Topopah Spring Tuff. Several pumping tests were conducted in borehole UZ-14 and drawdown was completely recovered after 5.6 days (Burger and Scofield, 1994; Cazarnnecki, 1995; and Luckey, 1993). This suggested that there may exist an extensive perched water body around this area. The perched water zone encountered in UZ-14 is at approximately the same stratigraphic level as the zone in UZ-1. This suggests that the same perched water body was encountered in both boreholes.

7.3.1.2 Borehole NRG-7a

Borehole USW NRG-7a is located in Drill Hole Wash at a surface elevation of 1,282 m. The borehole was drilled to a total depth of 461 m into the top of the Calico Hills Tuff. Perched water was reached between 458 and 461 m depth, just below the contact of the bedded tuff below the partially welded pyroclastic flow at the base of the Topopah Spring Tuff. The perched water was located near the contact of a series of highly fractured welded tuffs overlying relatively unfractured, nonwelded tuffs. As in the case with boreholes UZ-1 and UZ-14, the perched water may be entrapped in fractures where water is slowly imbibing into the matrix of the less permeable, underlying rock units.

7.3.1.3 Borehole SD-7

The perched water in SD-7 was found in the bottom portion of the Calico Hills zeolitic unit at a depth of 480 m, at an elevation of 880 m, and was 150 m above the regional water table (Soeder, 1995). Borehole USW SD-7 is located near the southwest corner of the ESF, just west of the Ghost Dance fault. The offset in the geologic layering due to the fault is estimated to be on the order of tens of meters. Preliminary analysis of hydraulic test data indicates that the volume of the perched water body appears to be small (about 30,000 m³) (Luckey, 1995) since the water level did not recover to the pre-pumping levels after testing. The Ghost Dance fault appears to block moisture which is being laterally diverted by an eastward-dipping portion of the zeolitic Calico Hills tuff to create the perched water body.

7.3.1.4 Borehole SD-9

Borehole USW SD-9 is located adjacent to Drill Hole Wash at a surface elevation of 1,302 m and has a total depth of 678 m. The perched water was found at a depth of 413 m, about 3 m above the lower nonlithophysal/vitrophyre contact in the Topopah Spring Tuff, and about 157 m above the water table. The perched water zone was near the upper contact of the basal vitrophyre of the Topopah Spring Tuff and was in highly fractured, welded tuff underlain by less-fractured, non-welded tuff.

7.3.2 Chemistry and Ages of Perched Water

A number of isotope analyses are being performed on perched water samples, matrix pore water samples, and matrix rock samples obtained from the unsaturated zone at Yucca Mountain. Perched water samples were collected and analyzed for boreholes UZ-1, UZ-14, SD-9, NRG-7a, and SD-7 (Rousseau et al., 1996; and Yang et al., 1996). Most of these samples were in the upper Calico Hills Formation, except those of UZ-14, which were from the bottom of the Topopah Spring Tuff.

Preliminary isotope data from UZ-14 and SD-7 perched water samples indicate that the water had about 28% modern ^{14}C , with an apparent residence time since infiltration of 10,800 years. The corrected age was within the 5,000 to 10,800 year range, and the samples may be a mixture of different ages (Yang, 1996). However, Fabryka-Martin and Liu (1995) found ^{36}Cl signals measured in the SD-7 and UZ-14 perched water samples ranging from present-day background to about 40% above background, indicating either the influence of a bomb-pulse or historically elevated ^{36}Cl levels. Saturated zone samples all had signals at or slightly below the present-day background level, consistent with groundwater travel times of less than 50,000 years.

Tritium measurements of UZ-14 and SD-7 samples gave similar results (Yang et al., 1996). They were not as depleted as would be expected from glacial-period recharge, but were more depleted than modern precipitation. This means that the water may have been a mixture of glacial and post glacial recharge. No bomb pulse signals were found in any of the borehole perched water samples when they were examined for ^3H .

When perched waters from these two boreholes were tested for Sr isotopic composition, UZ-14 samples gave values resembling those of pedogenic calcite. SD-7 samples had results similar to samples from the regional saturated zone. Testing for U isotopes produced similar conclusions. Based on these data, one hypothesis is that the UZ-14 perched water sample results are due to relatively local infiltration, while the SD-7 samples could be a remnant of the historic water table elevation during a period of high recharge. In opposition to this, however, is the relatively low chloride concentrations of 4-5 mg/l measured in SD-7 perched water (Fabryka-Martin and Liu, 1995). These low concentrations are consistent with an hypothesis of water infiltrating fairly soon after intense rainfall events. For comparison, samples from UZ-14 showed Cl concentrations of 7 mg/l. Samples from NRG-7a had concentrations of about 9-10 mg/l, while the average Cl concentration in local rainwater is about 0.5 mg/l.

Chemical and isotopic compositions of perched water shows that their major ion chemistry is similar to that of saturated zone groundwater. However, perched water from UZ-14 is close in composition to water from the Topopah Spring Tuff. Chloride concentrations in perched water are consistent with recharge through fractures and with little contribution from the pore water in the matrix of the overlying rock. The apparent ^{14}C residence times of perched

water are similar to those for Calico Hills formation pore water from UZ#16, ranging from 3,000 to 7,000 years (Rousseau et al., 1996).

7.4 Conceptual Model

Perched water may occur where large permeability differences exist between adjacent geologic formations. Perched water zones have been encountered in a number of boreholes at Yucca Mountain, as summarized in Section 7.3. The locations of boreholes important to the discussion of perched water are shown in Figure 7.3.1.1.

Identification of perched water zones at Yucca Mountain is complicated by the few field data and by the presence of the apparent hydraulic gradient which exists between boreholes near Yucca Wash and those located in the vicinity of Drill Hole Wash. The water table measured in boreholes G-2 and WT-6 is almost 300 meters higher than that in many of the other Yucca Mountain boreholes. However, some scientists have proposed that the gradient may actually be related to measurements of the top surface of a large perched water body recharged from the area north of Yucca Wash. Evidence supporting this concept includes a consistent small decrease in water table elevation since the mid-1980's and observation of water flow in fractures above the apparent water table (Czarnecki, 1995), as well as measurements in core samples from below the water table which are less than fully saturated. Pump tests are presently being conducted at borehole G-2 to investigate this hypothesis. Additionally, perched water zones at Yucca Mountain may have been enlarged significantly by the use of water as drilling fluid in the G-series boreholes. For instance, drilling fluid from borehole G-1 was found in samples obtained from the perched water zone at UZ-14.

Another complicating factor in identifying perched water is that the relatively uniform water level elevations measured in the vicinity of the repository area may actually be the potentiometric surface of a confined aquifer. This would explain why less-than-saturated conditions are found in core samples below the apparent water table. The interaction between the regional water table gradient, the perched water bodies, and the possible confined aquifer with an as yet unknown confining layer is not well understood at this time.

The perched water bodies or wet layers in these boreholes were detected in zones in or overlying geologic units which are extensively altered to zeolites. Alteration is often encountered in the material underlying the densely welded and fractured TSw. The importance of fractures to water movement through the tuff at Yucca Mountain is shown by the data recorded during drilling of UZ#16. Drillers report encountering a zone in the Prow Pass Tuff which provided dripping wet core samples below the expected potentiometric surface (Luckey, 1996). This zone was underlain by a zone which provided dry core samples, fol-

lowed by another zone yielding dripping wet cores. Flowing water was then encountered in a zone of fractures within a sequence of relatively unfractured rock. When the fractured zone was encountered, the water level in the borehole rebounded up to the predicted potentiometric surface.

Figure 7.4.1 shows the elevations of the perched water level from all of the boreholes discussed above, projected onto a north-south cross-section. The figure also indicates the top elevation of the nearest underlying zeolitic layer in the borehole. It shows the importance of the altered units with the perched water zones.

Figure 7.4.1

Perched water locations projected to a N-S cross-section their and relationships with vitric and zeolitic unit boundaries.

A contour map of the thickness above the water table of the surface where zeolites are first encountered below the base of the TSw, is given in Figure 7.4.2. Assuming that the zeolitic surface serves as a barrier to vertical flow and causes lateral diversions and perching, the figure shows that perched water north of Drill Hole Wash would be diverted in a southerly direction until it encounters a minimum along the alignment of Drill Hole Wash. Moisture flow south of Drill Hole Wash would be diverted in an easterly direction unless it is blocked by the Ghost Dance fault near the Bow Ridge fault. The bottom of the TSw is below the measured potentiometric surface, which means that fracture flow in the TSw in this region can reach the water table without moving through an extensively altered zeolitic layer.

Figure 7.4.2
Contour map of the thickness of zeolites above water table and below the base of the TSw, indicating possible flow paths and lateral diversions.

In the southern portion of the potential repository area and south of it, parts of the Calico Hills Formation and the Prow Pass Tuff are vitric. The first altered unit which could serve as a barrier to vertical flow is the lower Prow Pass. However, this layer is reported to be less altered than the Calico Hills Formation and may not impede or laterally divert flow to the same extent as the Calico Hills altered pyroclastic layers. Saturation profiles for the lower Prow Pass in borehole SD-7 show that saturations average about 95% while those of the altered Calico Hills Formation are close to 100%. Figure 7.4.2 shows a contour map of the thickness above the water table for the lower altered Prow Pass surface. The slope of this surface is generally easterly. The devitrified upper Prow Pass intercepts the water table in the vicinity of UZ-16. If vertical moisture flow is diverted laterally by the lowered altered layer and if the Ghost Dance Fault does not block the flow or provide an alternate pathway to the potentiometric surface, then lateral flow in the devitrified layer will reach the surface in that region without proceeding through a zeolitic layer. Data indicate that no perched water was found overlying the lower altered Prow Pass layer in this

borehole, which means that the layer is insufficiently altered to perch water, or that in this region the Ghost Dance fault is not blocking laterally diverted flow, or that the Ghost Dance fault is serving as an alternate pathway to the potentiometric surface.

The conceptual model used in this study is based on the current site-scale model grid and the geological model. The perched water bodies, near boreholes UZ-1/14, SD-9 and NRG-7a in the North Ramp area, were assumed to lie along the base of the TSw unit, a zone of more intensely fractured rock of the lower nonlithophysal zone. The water is perched upon less intensely fractured bedded tuff which is altered. This conceptual model is similar to the one discussed by Rousseau et al. (1996). However, the possible lateral barrier, or a northeast trending fault mentioned in that study, is not included explicitly in this study. The lateral water movement along or above the perched water bodies were simulated by: 1) ignoring the effects of fracture flow and 2) reducing both vertical and horizontal matrix permeabilities by several orders of magnitude. For the perched water near SD-7, the water body is considered to be located within the zeolitic unit.

7.5 Development of the Perched Water Model

7.5.1

Modeling Approach and Model Description

We performed a series of numerical simulations using three separate but related 3-D models to simulate the perched water occurrences in the unsaturated zone at Yucca Mountain. Two of the three models are based on the current site-scale model grid and the other is a smaller 3-D model extracted from the 3-D site-scale model. The site-scale model domain is shown in Figures 7.3.1.1 and 7.5.1.1. The total surface area covered by the site-scale model is approximately 37 km². Figure 7.5.1.1 also shows the model domain of the sub-model, a sub-set of the site-scale model grid around boreholes UZ-1/14, SD-9 and NRG-7a, and a plan view of the 3-D model grid. The site-scale model has 28 grid layers that represent different hydrogeological units and layers in the unsaturated zone of Yucca Mountain. Each grid layer, as shown in Figure 7.5.1.1, has 983 element blocks. The total number of element blocks in the grid is 26833. The sub-model, as shown in Figure 7.5.1.1 has 141 blocks per grid layer and 3752 element blocks.

Figure 7.5.1.1

A plan view of the site-scale model grid and the sub-model domain for perched water studies.

Perched water is generally a local phenomenon within the mountain, and it has been created due to the local heterogeneity and contrasts in permeability and geological structures of the fractured and unfractured tuffs. The perched water zone development is also dependent on sufficient water recharge from the ground surface over a long period of time. To simulate and predict perched water zones at the site accurately, we need more site-specific data, such as fracture and matrix properties and their detailed spatial distributions, formation layering information, and fault properties. In depth modeling studies of perched water are presently limited by the uncertainties in the site specific data and intensive computational requirement if much more refined grids of 3-D grid models are needed. Under the same limitations, the current 3-D site-scale model has been primarily used to estimate the movement of moisture and gas, and to provide understanding of the ambient geological and geothermal conditions at the mountain on a large scale. The spatial discretizations of the 3-D grid are relatively coarse with block size on the order of 10 to 100 meters. When the current 3-D model is applied to a perched water problem, the minimum water body predicted by the model will be at least the size of a single grid block, which may be too big for some actual small perched water regions.

In this report, we will present our simulation results of perched water obtained so far using the three 3-D models. The simulation results presented here were conducted using the TOUGH2 code (EOS3 module) under two-phase flow and non-isothermal conditions. The predicted perched water locations and volume of the model correspond to steady-state simulations of the 3-D models, under given infiltration and other boundary conditions, as discussed below. The modeling approach for treatment of fracture/matrix flow uses the generalized ECM formulation, as discussed in Chapter 4 (Wu et al., 1996).

The perched water bodies currently found at Yucca Mountain are the result of water movement through the mountain and surface infiltration at least during the last 5-10 thousands of years. Under such a large time scale, the perched water occurrence at Yucca Mountain can be reasonably approximated assuming steady-state or near steady-state conditions. Additional uncertainties are associated with the infiltration rate in the past, and modeled past infiltration rates may be used for transient simulations to look at current perched water conditions. This may introduce more unknowns to the predictions because of the uncertainties in the past infiltration history. Even though many other modeling approaches, such as dual-permeability, double- or multi-porosity methods, can be also used to investigate fracture/matrix flow and its relation to perched water occurrences, the ECM model has proven to be simple in data requirement, computationally efficient, and accurate in solutions as well. A systematic study of comparisons of different model approaches to treat fracture/matrix flow has been conducted at LBNL this year. The results of the study indicate that the generalized ECM approach gives almost identical solutions to model-predicted moisture flow variables of matrix and fracture, when compared with those from the dual-permeability or multi-porosity models under steady-state or near steady-state conditions (See Chapter 6 for 1-D model, Chapter 12, for 2-D model and Chapter 8 for 3-D comparison studies).

7.5.2 Boundary Conditions and Model Parameters

For the three 3-D perched water model, the boundary conditions, data specifications, and rock properties used are specified as below:

The ground surface is taken as the top model boundary, and the water table is treated as the bottom boundary. Both of these model boundaries are treated as Dirichlet-type conditions, i.e., constant (but distributed) temperatures, constant (but distributed) gas pressures and constant liquid saturation are specified. The constant values of temperatures on the boundaries are determined based on the field observation data, as described in Chapter 8 (Wu et al, 1996). The gas pressures at the bottom boundary are calculated using the observed gas pressure and relative elevations to the observation point. The surface gas pressures are simulated by running TOUGH2 to steady-state under given temperature, infiltration and bottom pressure conditions.

A spatially distributed net infiltration map (Hevesi and Flint, 1995), as shown in Figure 7.5.2.1, with an average rate of 0.35 mm/yr over the site-scale

model domain has been specified at the top boundaries of two of the 3-D models. The figure shows higher infiltration rates at the northern part of the model domain and along the south-north ridge of the mountain. Much lower infiltration can be seen along or near the Bow Ridge fault (Figure 7.3.1.1), the eastern part, and near the south west corner of the model area. The other infiltration map recently received from USGS (Flint et al., 1996) is also going to be used for our perched water modeling studies.

Figure 7.5.2.2 shows the net infiltration map over the site-scale model domain. The average infiltration rate is 4.4 mm/yr, which is more than ten higher than that shown in Figure 7.5.2.1. But the spatial distribution of infiltration in both figures is very similar, with higher values in the north part of the model domain and along the mountain ridge from south to north. Since we received this newest infiltration map very recently, the simulation study of perched water using this higher infiltration rate is still underway, and we will report the final results in a later report.

Figure 7.5.2.1
Net infiltration map (Map #1) showing infiltration rates and distributions over Yucca Mountain (Hevesi and Flint, 1995).

Figure 7.5.2.2

Net infiltration map (Map #2) showing infiltration rates and distributions over Yucca Mountain (Flint et al., 1996).

All the model input data parameters, properties of rocks (fracture and matrix) and fluids, hydrogeological units, and soil characteristic curves were the same as those used in the site-scale model, as discussed in Chapter 3 (Bandurraga et al., 1996) and Chapter 8 (Wu et al., 1996). The rock properties used for matrix and fractures were estimated using the ITOUGH2 code (Finstlerle, 1993) based on the QA saturation and water potential data as initial estimations (see Chapter 3, Bandurraga et al., 1996 for details), except for the permeabilities and capillary functions at and near perched water zones. In the perched water zone, matrix permeability and capillary pressure were calibrated as discussed below. The rock properties of matrix and fractures used are listed in Table 7.5.2.1.

Perched Water Analysis

Table 7.5.2.1 The rock properties of matrix and fractures for perched water studies.						
Units	k_m (m ²)	k_f (m ²)	α_m (Pa ⁻¹)	α_f (Pa ⁻¹)	m_m	m_f
tcw11	0.179E-19	0.519E-11	0.351E-05	0.235E-03	0.414	0.585
tcw12	0.104E-15	0.576E-11	0.226E-05	0.596E-03	0.486	0.412
tcw13	0.116E-17	0.621E-11	0.351E-05	0.776E-04	0.545	0.501
ptn21	0.181E-14	n/a	0.253E-04	n/a	0.206	n/a
ptn22	0.504E-14	n/a	0.150E-04	n/a	0.138	n/a
ptn23	0.126E-13	n/a	0.200E-04	n/a	0.240	n/a
ptn24	0.126E-13	n/a	0.2 86E-04	n/a	0.344	n/a
ptn25	0.362E-14	n/a	0.376E-04	n/a	0.263	n/a
tsw31	0.385E-16	0.249E-11	0.125E-04	0.306E-03	0.368	0.294
tsw32	0.276E-16	0.962E-11	0.751E-05	0.611E-04	0.243	0.254
tsw33	0.636E-18	0.483E-11	0.251E-05	0.110E-03	0.333	0.418
tsw34	0.359E-17	0.479E-11	0.667E-06	0.876E-04	0.552	0.459
tsw35	0.179E-18	0.497E-11	0.173E-05	0.921E-04	0.289	0.419
tsw36	0.322E-18	0.457E-11	0.592E-06	0.611E-04	0.387	0.399
tsw37	0.669E-16	0.409E-11	0.735E-06	0.114E-03	0.464	0.438
ch1vc	0.602E-11	0.723E-12	0.157E-05	0.240E-03	0.469	0.518
ch2vc	0.199E-11	0.723E-12	0.320E-05	0.240E-03	0.554	0.742
ch3vc	0.199E-11	0.723E-12	0.320E-05	0.240E-03	0.554	0.742
ch4vc	0.199E-11	0.723E-12	0.320E-05	0.240E-03	0.554	0.742
ch1zc	0.114E-14	0.100E-12	0.251E-06	0.735E-04	0.505	0.518

Table 7.5.2.1 (cont.) The rock properties of matrix and fractures for perched water studies.						
ch2zc	0.266E-17	0.560E-13	0.547E-06	0.755E-04	0.319	0.321
Units	k_m (m ²)	k_f (m ²)	α_m (Pa ⁻¹)	α_f (Pa ⁻¹)	m_m	m_f
ch3zc	0.266E-17	0.560E-13	0.547E-06	0.755E-04	0.319	0.321
ch4zc	0.741E-20	0.121E-12	0.103E-05	0.365E-04	0.489	0.639
pp3vp	0.279E-11	0.300E-13	0.900E-05	0.133E-03	0.363	0.467
pp2zp	0.956E-16	0.654E-13	0.823E-05	0.372E-03	0.213	0.206
bf3vb	0.279E-11	0.300E-13	0.900E-05	0.133E-03	0.363	0.467
bf2zb	0.956E-16	0.654E-13	0.823E-05	0.372E-03	0.213	0.206
tm3vt	0.279E-11	0.300E-13	0.900E-05	0.133E-03	0.363	0.467

where k_m and k_f are saturated matrix and fracture continuum permeabilities; α_m and α_f are van Genuchten's parameter of capillary pressure of matrix and fracture; and m_m and m_f are van Genuchten's parameter of soil retention curves.

Uniform fault properties are specified for all the incorporated faults shown in Figure 7.3.1.1. Matrix permeability of 100 md is used for faults, and horizontal and vertical permeabilities for fractures in faults are 10 and 100 darcies, respectively. For fault zones, $\alpha_m = 0.61E-4$, $\alpha_f = 1.0E-3$, $m_m = 0.5$, and $m_f = 0.5$, with the units in Table 7.5.2.1.

The values of rock permeability and van Genuchten parameters for grid blocks near or below the identified water bodies were adjusted to create water-trapping conditions there. However, all the adjusted permeabilities were generally within the ranges of observed or laboratory measured values.

As listed in Table 7.5.2.1, the rock parameter specification in the 3-D site-scale model is by layers, but some zones are located for grid layers in the CHn unit for vitric or zeolitic. In these layers zeolitic and vitric tuff properties are specified for corresponding geologic units, instead of layer-wise specification. The whole formation system is subdivided, in general, into 28 hydrogeological units. We have conducted a systematic sensitivity study using 1-D and 3-D sub-models and theoretical analysis to investigate water perching conditions at the mountain. We have found that it is necessary to make some local modifications

in rock properties in order to produce water perching conditions using the model, i.e.; in the same grid layers, different rock properties were used for different areas. The detailed information about rock parameters and their adjustments made in the 3-D simulations will be discussed in the following section.

7.5.3 Results and Analyses

The basic feature of a perched water body is that there exists a high water content region in a vadose zone, and the porous and fractured rock within this zone are fully or nearly fully water saturated. Substantial fracture flow may be initiated by a perched water body if in a welded unit. The capillary forces or water potentials become very small or even positive under fully saturated condition. The water perching conditions may also be established under certain two-phase conditions when there exists a residual or trapped gas saturation. In this case, the system will never become completely liquid saturated, and the local water potential, or pressure heads are always negative. However, as liquid content builds up and the air phase becomes trapped, isolated and immobile, both water and gas pressures increase locally. Once the local water pressure reaches a threshold value, such as static atmospheric gas pressure at the location (if no perched water were to exist), water will seep out from the fractures or pores when a borehole or tunnel happens to intersect this zone. From the modeling point of view, a perched water zone may be established when water saturation is high enough and capillarity is sufficiently small in a zone above the regional water table.

In our 3-D model, each borehole with perched water occurrence can be represented using the corresponding rock columns from the 3-D site-scale model grid. The simulation results can be analyzed in terms of saturation and water potential profiles. However, boreholes UZ-1 and UZ-14 are so close to each other that we use a single grid column (# 425) to represent them. Borehole NRG-7/7a is represented by column # 146, SD-9 by column # 507, and SD-7 by column # 221 of the 3-D model grid.

We also developed four vertical cross-sections to analyze the 3-D model results. Their locations are shown in Figure 7.5.3.1. Section W-E (UZ-14) crosses UZ-14 from west to east, and Section S-N (UZ-14) crosses south to north. Cross Sections W-E and S-N (SD-7) cross SD-7 going from west to east and south to north, respectively.

Figure 7.5.3.1
Locations and plan view of four vertical cross sections and associated boreholes.

Based on our series of modeling and theoretical analyses, we have found that a water perching (or trapping) condition in the unsaturated zone of Yucca Mountain is difficult to construct using a three-dimensional grid, representative geological information and realistic hydrogeologic properties. The difficulties are due to the lack of understanding of the physics behind the perched water occurring at the site, due to the lack of field data or studies since all the perched water observations were found by accident, and also related to the tremendous numerical problems associated with two-phase and 3-D flow in a heterogeneous system. Under these flow conditions it is relatively easy to create a high saturation zone in a model, but it is very difficult to create both high liquid saturations and positive water heads using the rock characteristic curves given. There are three necessary conditions for a perched water zone to develop, including (1) water-trapping geological structures, surrounded and underlain by very low permeability layers with few connected fractures or by capillary barriers; (2) low capillary suction forces in the rock under high saturation conditions within and near the perched water body, and (3) sufficient high infiltration rates over the mountain.

Perched Water Analysis

For the perched water zone around UZ-1/14, SD-9 and NRG-7a, the matrix rock properties were adjusted in order to create a water perching condition in this area using the 3-D model grids. The three grid layers with adjusted rock properties were tsw37, ch1zc, and ch2zc (see Table 7.5.2.1), which are the bottom layer of TSw, and the top two layers of the Calico Hills zeolitic unit. In the model output, the names of the material were changed to pch37, pch1z, and pch2z for convenience in the model input. The material boundary of the modified zone is bounded by the sub-model domain (Figure 7.5.1.1). Also in these three parameter-adjusted grid layers, effects of fractures on global moisture movement are ignored, and the rock within these layers is treated as a single porous medium. The other important modification to the rock properties in the perched water zone is that we introduce residual gas and satiated saturation mechanisms to account for the trapped air phenomena in the rock matrix. Under such conditions, gas phase becomes immobile and capillary pressure reduces to very small or zero when gas saturation is below its residual value. Also, the Corey's relative permeability functions are used for gas flow in these layers instead of van Genuchten's correlation. The capillary and water relative permeability functions, i.e. van Genuchten's functions, were used. The calibrated matrix rock properties are listed in Table 7.5.3.1.

The simulation results discussed in this section were obtained using the TOUGH2 code, the two 3-D model grids, the above-discussed boundary and infiltration conditions, and the rock properties given in Tables 7.5.2.1 and 7.5.3.1. The perched locations were analyzed using steady-state simulation results, and pumping test analysis was based on transient solutions.

Table 7.5.3.1 The calibrated rock matrix properties for perched water studies in the vicinity of UZ-1/14, SD-9 and NRG-7a.				
Units	k_m (m^2)	α_m (Pa^{-1})	S_{gr}	S_{ls}
pch37	0.669E-18	0.735E-07	0.02	0.98
pch1z	0.114E-18	0.251E-07	0.02	0.98
pch2z	0.266E-18	0.547E-06	0.02	0.98

In Table 7.5.3.1, k_m is adjusted matrix permeability; α_m is adjusted van Genuchten parameter of capillary pressure; S_{gr} is residual gas saturation; and S_{ls} is satiated liquid saturation.

The perched water near SD-7 is located within the zeolitic grid layers, ch2zc and ch3zc, within the zeolitic units of the CHn formation. The matrix rock properties used for this perched water zone were estimated by the ITOUGH2 code, and are listed in Table 7.5.3.2. The ITOUGH2 estimation was based on the infiltration map #1 (Figure 7.5.2.1) (see Chapter 3 or 8 for details).

Perched Water Analysis

Table 7.5.3.2 The calibrated rock matrix properties for perched water studies in the vicinity of SD-7.		
Units	k_m (m^2)	α_m (Pa^{-1})
ch3zc	0.428E-17	0.432E-06
ch4zc	0.871E-20	0.130E-05

7.5.3.1 Comparisons with Measured Borehole Data

As a first step for perched water calibrations of the site-scale model, saturation and water potential data are used to compare with the model predictions. Figure 7.5.3.2-7.5.3.5 show comparisons of the simulated and observed saturation and capillary pressure (water potential) data for boreholes UZ-1/14, NRG-7a, SD-7, and SD-9. The modeled results are from the 3-D site-scale model simulations. As shown in the figures, the observed saturation and water potential values are selected from the measured data when available (OCRWM/DOE, 1995b). The simulation results are generally in good agreement with the measured saturation profiles, but comparisons with capillary pressure data are not as good as those for saturation. The reason for this discrepancy in capillary pressure comparisons may be due to the inaccuracy in the measurement of these water potentials from sample handling to laboratory experiments, and due to the coarse grid and the conceptual model used. Also, there are no measured water potential data for the NRG-7a borehole.

Figure 7.5.3.2
Comparisons of the simulated and observed values for perched water in Borehole UZ-1/14;
(a) saturation, (b) capillary pressure.

Perched Water Analysis

Figure 7.5.3.3

Comparisons of the simulated and observed values for perched water in Borehole NRG-7a;
(a) saturation, (b) capillary pressures.

Figure 7.5.3.4

Comparisons of the simulated and observed values for perched water in Borehole SD-7;
(a) saturation, (b) capillary pressures.

Figure 7.5.3.5
Comparisons of the simulated and observed values for perched water in Borehole SD-9;
(a) saturation, (b) capillary pressures.

Figure 7.5.3.2 shows comparison of the simulated and observed saturations and capillary pressures water potentials for boreholes UZ-1/14, indicating a reasonable agreement. Especially, a good correlation exists for saturations in all four units of the Tiva Canyon, Paintbrush, Topopah Spring, and Calico Hills. At the perched water location of about 960 m elevation in the two boreholes, the simulated water saturations are at 1 and water potential reduces to 0, respectively. This implies that in this case, perched-water conditions are created by the model, and simulated results also match the perched water elevation, as circled in the figure.

Figure 7.5.3.3 shows the simulation results for the NRG-7/7a borehole, and the comparison is only for the saturations, because there are no measured in situ data for water potential from this borehole. The simulated water saturation profile is in fair agreement with the observed values. The figure shows that the simulated saturation profile is a little "wetter" than observed. This may be due to the quality of the measured data, because the sample cores taken from the borehole were not handled properly and some moisture may have been lost (Flint, 1996). The computed perched water elevation is close to the high saturated zone of the observation, as indicated by the figure. The simulated saturations at the perched water level are close to one, and the water potentials are lower there.

Figure 7.5.3.4 gives the results for borehole SD-7. The comparisons of the simulated and observed saturations and capillary pressures are good. Different

Perched Water Analysis

from all the other boreholes discussed in this report, the perched water body found in SD-7 is located within the Calico Hills zeolitic unit, rather than at the bottom of the welded tuff layer of Topopah Spring unit. As shown in Figure 7.5.3.4, the perched water location is reproduced well by the 3-D model. Higher saturations and lower water potentials are given by the model at the perched water level in this borehole.

Figure 7.5.3.5 presents the results for borehole SD-9. The overall agreement between the modeled and observed saturations is very good considering the relative coarse grid used in the 3-D model. The computed perched water location matches the field data well.

7.5.3.2 Simulated Perched water Bodies

Figures 7.5.3.2 - 7.5.3.5 show the observed and simulated perched water elevations in the four boreholes. However, the simulated perched water bodies and their sizes can be more clearly depicted in plan or in vertical cross sections. The computed results, obtained from the 3-D runs, are given in the following sections.

Perched Water Zone for UZ-1/14, SD-9 and NRG-7A

Figure 7.5.3.6 shows water saturation contours in plan view along the base of the Topopah Spring unit, indicating clearly a perched water body by boreholes UZ-14, SD-9 and NRG-7a. The circle drawn around UZ-14 with near fully saturated conditions has a radius of about 600 meters. The perched water body by UZ-1/14 may extend further to the north or to borehole G-2, which is not indicated in the figure and needs further investigation. It is also interesting to note in the figure that relatively higher saturation values exist in the northern part of the model domain where the higher infiltration rates occur (see Figures 7.5.2.1). Figure 7.5.3.6 also shows lower saturations along the major faults, which is due to higher permeability and lower capillary suction forces in the fault zones.

Figure 7.5.3.7 gives the capillary pressure distributions at the same elevation as in Figure 7.5.3.6. Again very low capillary forces can be seen in the perched water zone around UZ-14, SD-9 and NRG-7a. Actually the simulated water pressure at the base of TSW unit of perched water zones are 2-3 bars, and single-phase water flow conditions are created by the model. It should be mentioned that higher capillary pressures are noted to the southern part of the model domain or near south-west model boundary, except within the fault zones. Figures 7.5.3.6 and 7.5.3.7 show that the simulated perched-water zone extends between boreholes UZ-1/14, SD-9, and NRG-7a.

Figure 7.5.3.6

A plan view of saturation contours in the base of TSW showing the perched water body around UZ-1/14, SD-9 and NRG-7a.

Figure 7.5.3.7

A plan view of capillary pressure contours in the base of TSW showing the perched water body around UZ-1/14, SD-9 and NRG-7a.

Figure 7.5.3.8

Liquid saturation along the West-East section crossing borehole UZ-1/14

In order to observe the vertical distribution of the perched water bodies, four vertical cross sections are drawn through UZ-14 and SD-7, from west to east, and south to north, respectively (see Figure 7.5.3.1). Figure 7.5.3.8 shows the water saturation distributions along the west-east section crossing UZ-14. As can be seen in this figure, there is an extensive water body near borehole UZ-14 around the observed perched water location. Water saturations along the south-north direction are given in Figure 7.5.3.9 which also shows that there exists a large perched water zone, especially to the north of UZ-14.

Figure 7.5.3.9
Liquid saturation along the South-North section crossing borehole UZ-1/14.

Perched Water Zone for SD-7

Figure 7.5.3.10 depicts the simulated perched water body along the west-east vertical cross section intersecting SD-7. The figure shows a very small perched water volume located within the Calico Hills zeolitic unit and abutting against the Ghost Dance fault. However, in the south-north direction, parallel to the Ghost Dance fault, the simulated high saturation zone appears to be extensive, but relatively thin along the lower permeable zeolitic layer (Figure 7.5.3.11). The perched water conditions, dependent on the local rock properties, may not develop further to the north along the zeolitic layer from SD-7, since no perched water was found for SD-12. The perched water found in borehole SD-7 is created in the model due to the less permeable underlying layer and the fault, which in this case serves as a capillary barrier. The areal extension of the SD-7 perched water body is also controlled by the surrounding more permeable, vitric formation, especially to the west of Borehole SD-7 (Figure 7.5.3.10).

Figure 7.5.3.10
Liquid saturation along the West-East section crossing borehole SD-7.

Figure 7.5.3.11
Liquid saturation along the South-North section crossing borehole SD-7.

Figure 7.5.3.12

Three-dimensional saturation distributions, indicating the higher saturation zones for the perched water bodies.

Figure 7.5.3.13

Three-dimensional capillary pressures, indicating the lower capillary in the perched water bodies.

Perched Water Analysis

3-D view of Perched Water Zones

A perspective view of 3-D liquid saturation distribution within the unsaturated zone of Yucca Mountain is shown in Figure 7.5.3.12 for saturations and 7.5.3.13 for capillary pressures. A large perched water body is clearly indicated by higher water saturations and lower capillary pressures near UZ-1/14 and SD-9. South to this perched water zone along the ESF, a thin water body appears within the Calico Hills unit and intersects with borehole SD-7.

7.5.3.3 Pumping Test Analysis of UZ-14

Several hydraulic pumping tests have been conducted in the perched water boreholes at Yucca Mountain (Luckey, 1993; and Soeder, 1995) to study perched water occurrences in the area. Some of these tests have provided useful information on the nature of the perched aquifers. The most successful pumping tests may be those conducted in UZ-14, and we will use data from two of these tests and the 3-D sub-model in our analysis.

According to Luckey (1993), four hydraulic pumping tests were conducted on UZ-14 between August 17 and 27, 1993. However, only two of them were successful (tests #2 and #4). As summarized in Section 7.3, the perched fluid in UZ-14 was encountered at 383 m depth, in the lower nonlithophysal unit of Topopah Spring. The static fluid level was at about a depth of 381 m, or at an elevation of 968 m. In test #2, conducted on August 19, 1993, water was pumped for 13 hours from the borehole at a rate of 0.90 gal/min. The water level was continuously monitored for 20 more hours after pumping stopped. Test #4 started on August 24, 1993; pumping lasted for more than 66.8 hours at a rate of 0.93 gal/min, and the water level in UZ-14 was monitored for 3 more days. During the four tests, the total water volume extracted was 6,190 gal. and total pumping time was 102.2 hours. The water level fully recovered in about 5.6 days.

In order to analyze the pumping tests using a 3-D numerical method with a spatially discretized grid, mesh size must be fine enough to obtain acceptable resolutions in the results. This is why we need to use a submodel with a local refined (R-Z) mesh around UZ-14. Since the sub-model uses the same size grids as in the 3-D site-scale model grid of Section 7.5.1, we used a local refined R-Z mesh which is connected to the perched water layer and UZ-14 (tsw37 or pch37) in the model. The local refined, embedded R-Z grid is centered at UZ-14 with an inner borehole radius of 12 1/4 inches. Many numerical runs were conducted to match the results of the two pumping tests, and we found that certain modifications to the refined R-Z meshes and their properties were necessary to fit both water drawdown and recovery data. The calibrated parameters include the minimum volume of perched water and the local horizontal permeability. The local horizontal permeability is contributed by local fractures which connect with boreholes and provide local pathways for water flow between matrix and borehole, but do not contribute to the global flow between the layers. The calibrated results are: (1) the formation volume of the perched water zone is at least $4.5 \times 10^7 \text{ m}^3$ (or equivalent to a cylinder of formation with radius, $R=600\text{m}$, height, $Z=40 \text{ m}$); and (2) the formation hosting the perched water zone near UZ-

14 is radically heterogeneous with two different local horizontal permeabilities (i.e., $k = 250$ md for $R < 150$ m, and $k = 150$ md for $R > 150$ m).

The comparisons of the observed and simulated pumping test results are shown in Figures 7.5.3.14 to 7.5.3.19. We used linear-scaled, semi-log and Horner plots to analyze the pumping data.

Figures 7.5.3.14 to 7.5.3.16 show plots of pumping test#2 results. Figure 7.5.3.14 indicates that there is an excellent agreement between the observed and simulated water levels. The water levels predicted by the model not only match during the drawdown period, but also during recovery (or buildup period) after pumping stopped. The data for the recovery period are shown on a semi-log plot in Figure 7.5.3.15. There is a good fit for the later buildup times, after 50 minutes of recovery. However, at early times (i.e., less than 20 minutes), the model does not match the observed water levels well. This may be due to well-bore storage, damage or skin effects. The corresponding Horner plot (Earlougher, 1977) is given in Figure 7.5.3.16, where T_p is the total pumping time, and Δt is the time since pumping stopped. The Horner curve of Figure 7.5.3.16 also shows that discrepancy exists at early times with a much better agreement at later times. Figures 7.5.3.15 and 7.5.3.16 also show that the model gives similar slopes on the semi-log plots at later times. This indicates that the adjustments in the local horizontal permeability near the borehole is reasonable.

Figure 7.5.3.14
Comparison of the observed and simulated water levels for test#2 in borehole UZ-14 using a linear plot.

Figure 7.5.3.15
Comparison of the observed and simulated water levels for test#2 in borehole UZ-14, using a semi-log plot.

Figure 7.5.3.16
Comparison of the observed and simulated water levels for test#2 in borehole UZ-14 using a Horner plot.

Figure 7.5.3.17 Comparison of the observed and simulated water levels for test#4 in borehole UZ-14, using a linear scaled plot.

Figure 7.5.3.18 Comparison of the observed and simulated water levels for test#4 in borehole UZ-14, using a semi-log plot.

Figure 7.5.3.19

Comparison of the observed and simulated water levels for test#4 in borehole UZ-14, using a Horner plot.

Figures 7.5.3.17 to 7.5.3.19 present the pumping test and simulation results for pumping test #4 in borehole UZ-14. It should be mentioned that identical model parameters were used as before except for pumping rates and times. Figure 7.5.3.17 compares the observed and simulated water levels and shows a good agreement during the pumping period. The match during recovery is reasonable, but not as good as in test#2. This may be due to the much longer pumping period in test#4, 66.8 hours versus 13 hours in test#2. It is expected that for short-time pumping tests, the hydraulic behavior of the well is controlled by the nearby perched water body, and the flow towards the well is radial and horizontal. During longer pumping times, the pressure disturbance penetrates much deeper into the formation in all three directions. Therefore, some local, vertical fractures may also contribute significantly to the water level recovery. In our 3-D sub-model, we did not include vertical features that may control flow near the wellbore at later times. This may explain why there is a poor agreement between observed and computed water levels during the recovery period. The semi-log curve (Figure 7.5.3.18), and the Horner plot (Figure 7.5.3.19) for test#4 indicate a similar behavior as in test#2. During the very early recovery period, there is certain difference between the simulated and observed water levels. Better agreement is obtained at later times. However, the slopes in the semi-log plot are not in very good agreement at later times, which

may suggest that there may be strong three-dimensional flow effects during this period.

According to Luckey (1993), no boundary effects can be detected from the pumping test data. Based on this and the fact that the water level fully recovered in about 5.6 days, it has been speculated that the perched aquifer is extensive around UZ-1/14. Based on our pumping test analysis, we can estimate that the perched water volume is on an order of a million cubic meters, assuming a porosity of 5%. This value is close to that estimated by the North Ramp Report (Rousseau et al., 1996) of 645,000 m³.

7.6 *Current Studies Using the New Infiltration Map*

Our third perched water model is based on the site-scale model grid (Figure 7.3.1.1) and the newest infiltration map (Map # 2, Figure 7.5.2.2) from USGS (Flint et al., 1996). The infiltration map is being Q at the USGS. Work on perched water analysis using this new infiltration map is underway, and the final results will be reported in a later report. The new infiltration map shows a much higher infiltration rate in the North Ramp areas along the mountain ridge, with an average infiltration of 4.4 mm/yr over the model domain, which is more than ten times larger than the value shown on map # 1 (Figure 7.5.2.1). The preliminary simulation results indicates that using the new infiltration map will result in not only the right perched water locations, but also will match the ages of the water in the perched aquifers of UZ-1/14 and SD-7. The groundwater travel times based on particle tracking models are between 5,000 to 10,000 years, which are consistent with the isotope ages of 5,000 to 10,800 years (see Chapter 8, Wu et al., 1996).

7.7 *Conclusions*

One of the applications of the three-dimensional site-scale unsaturated-zone model is to predict and evaluate the hydrogeological conditions under which perched water zones will develop. The presence of perched water at Yucca Mountain has many implications and may have significant effects on the construction, operation and performance of the repository. The occurrence of perched water bodies in the unsaturated zone of Yucca Mountain indicates that currently in the area, water-trapping conditions exist. It also implies that the much higher infiltration rates over the mountain may have occurred in the past, and that there may exist preferential pathways for water to travel from the surface to the water table. Water diverted by the perched water zone may flow through fault zones or other higher permeable channels, bypassing the low permeability zeolitic units in the CHn down to the water table. As a result, a very non-uniform areal recharge is expected for the water table.

In this report, the relevant data on the perched water bodies at the Yucca Mountain site are collected and analyzed, a conceptual model of perched water occurrences is discussed, and computer modeling studies on perched water incidence at the site are described.

Three 3-D models were developed to investigate the localized perched water phenomenon at Yucca Mountain. Field data on perched water from 5 boreholes were discussed and used to calibrate the 3-D models in reproducing the water perching conditions in the unsaturated zone of the mountain. The 3-D steady-state simulations were conducted using an areally distributed infiltration map from USGS (Hevesi and Flint, 1995). Since the surface infiltration condition and the simulation studies using the newer infiltration map (Flint et al., 1996) are in progress, the results will be reported later. The constructed 3-D models are used to investigate the effects of matrix permeability variation of the welded and nonwelded tuffs. The only rock properties calibrated in this study were matrix permeabilities, capillary functions, and gas relative permeabilities within the perched water zones. The modified values were within the range of observed and laboratory tested values. The key factors in creating a perched water zone are: (1) a water perching geologic structure underlain or surrounded by low permeability zones, (2) weak rock capillary suctions under high saturation conditions within and near perched water zones, and (3) sufficient water infiltration rates.

The results of this steady-state modeling study are in agreement with the observed perched water data, in term of water saturation, potential profiles, and perched water locations. The three-dimensional models could reproduce the water perching conditions as observed in the boreholes. Furthermore, transient numerical modeling studies of the pumping tests were performed using a 3-D submodel for borehole UZ-14. The numerical results match well with the observed water level data. The perched water volume around UZ-1/14 is estimated to be about 1 million cubic meters.

The modeling studies reported in this chapter provide much confidence in the site-scale unsaturated zone model for incorporating the perched water data and investigating perched water occurrences at the mountain. However, there is still considerable uncertainties in our understanding of perched water occurrences at Yucca Mountain. Among these uncertainty are the problems with (1) the accuracy of simulating current and past net water infiltration rates over the mountain; (2) the estimation of matrix/fracture properties of rocks; (3) the quantitative description of heterogeneity of welded and non-welded tuffs, their flow properties and detailed spatial distribution within the site; (4) the lack in understanding water-trapping mechanisms in the perched zone of the mountain, such as the role played by trapped air, and capillary behavior in higher liquid saturations; and (5) the insufficient number of relevant field studies. Also, the importance to the model of the higher water gradient near the northern model boundary around borehole G-2 is not well understood. There is still a

need to refine the 3-D model grid around the potential perched water bodies for detailed modeling analysis.

Future modeling studies of perched water occurrences at Yucca Mountain should focus on: (1) incorporating distributed matrix/fracture rock properties; (2) using updated and more accurate geological models for different hydrogeologic units, especially for the highly contrasting vitric and zeolic zones and their spatial distributions; (3) using local refined numerical grids along the interface of those vitric and zeolitic units; (4) applying infiltration scenarios and hydrogeological conditions to predict water perching conditions and occurrences; and (5) the effects of thermal loading and air circulation on perched water development.

The observed liquid saturation and water potential data from borehole UZ-14, SD-9, NRG-7a and SD-7 are all Q data. These data were used for model calibration studies. Also, the perched water data from all of the boreholes are Q, except for that from UZ-1. The perched water from UZ-1 was used as corroborating data.

The computer codes used in this study are TOUGH2 and ITOUGH2. Both have been qualified for the study reported in this chapter.

7.8 References

- Burger, P.A. and K.M. Scofield, Perched water at Yucca Mountain – implications on the exploratory studies facility, Nye County, Nevada, Water-Resources Investigations Report, U.S. Geological Survey, Denver, CO, 1994.
- Czarnecki, J., Personal communication, 1995.
- Earlougher, Jr., R.C., Advances in well test analysis, Society of Petroleum Engineers of AIME, Monograph, v. 5, pp. 45-58, 1977.
ACCN: NNA.19900104.0471
- EG & G Energy Measurements, Remote Sensing Laboratory, Yucca Mountain Site Characterization Project, site atlas supplement, 1993.
- EG & G Energy Measurements, Remote Sensing Laboratory, Yucca Mountain Site Characterization Project, site atlas, 1994.
- Fabryka-Martin, J, and B. Liu, Distribution of chlorine-36 in UZ-14, UZ-16, perched water, and the ESF north ramp, Yucca Mountain, Nevada, Los Alamos National Laboratory Milestone 3431, Los Alamos National Laboratory, Los Alamos, NM, 1995.

Perched Water Analysis

- Finsterle, S., ITOUGH2 User's Guide, Version 2.2, Lawrence Berkeley National Laboratory Report LBL-34581, UC-600, Lawrence Berkeley National Laboratory, Berkeley, CA, 1993.
ACCN: MOL.19941026.0075
- Flint, L., Permeability Data for boreholes UZ-16 and SD-9, from Yucca Mountain, Nevada, U. S. Geological Survey, Denver, CO, 1995.
DTN: GS940508312231.006 Q
DTN: GS950608312231.005 Q
- Flint, L., Personal communication, 1996.
- Flint, A.L., J.A. Hevesi, and L.E. Flint, Conceptual and numerical model of infiltration for the Yucca Mountain Area, Nevada, U. S. Geological Survey, Water-Resources Investigation Report-96, Denver, CO, 1996.
- Freeze, R.A., and J.A. Cherry, Groundwater, Englewood Cliffs, N. J., Prentice-Hall, 1979.
ACCN: HQS.19880517.1763
- Hevesi, J.A. and A.L. Flint, Geostatistical model for estimating precipitation and recharge in the Yucca Mountain region, Nevada-California, U. S. Geological Survey, Water-Resources Investigation Report, Denver, CO, 1995.
DTN: GS960108312111.001 (Non-Q)
- Luckey, R.R., Update on fluid in USW UZ-14, Presented in the Nuclear Waste Technical Review Board Meeting, Las Vegas, NV, 1993.
ACCN: NNA.19931111.0085
- Luckey, R.R., Perched water testing - USW SD-7, Personal communication, March, 1995.
- Luckey, R.R., Personal communication, September, 1995.
- Luckey, R.R., Distribution of chlorine-36 in UZ-14, UZ-16, perched water, and the ESF North Ramp, Yucca Mountain, Nevada, Los Alamos National Laboratory Milestone 3431, Los Alamos National Laboratory, Los Alamos, NM, 1996.
- Luckey, R.R., Personal communication, April, 1996.
- OCRWM/DOE, Technical Data Catalog, Yucca Mountain Site Characterization Project, 1995a.
- OCRWM/DOE, Of Mountains & Science, Yucca Mountain Project, 1995b.

- Peterman, Z.E., J.S. Stuckless, B.D. Marshall, S.A. Mahan, and K. Futa, Strontium isotope geochemistry of calcite fracture fillings in deep core, Yucca Mountain, Nevada—a Progress Report, In Proceedings of the Third Annual International Conference on High Level Radioactive Waste Management, American Nuclear Society and American Society of Civil Engineers, Eds., Las Vegas, NV, V. 2, pp. 1582-1586, 1992.
ACCN: NNA.19921116.0073
- Pruess, K., TOUGH2 - a general-purpose numerical simulator for multiphase fluid and heat flow, Lawrence Berkeley Laboratory Report LBL-29400, Lawrence Berkeley Laboratory, Berkeley, CA, 1991.
ACCN: NNA.19940202.0088
- Pruess, K., A. Simmons, Y.S. Wu, and G.J. Moridis, TOUGH2 software qualification, Lawrence Berkeley Laboratory Report LBL-38383, Lawrence Berkeley Laboratory, Berkeley, CA, 1996.
- Rousseau, J.P., E.M. Kwicklis, and D.C. Gillies, Hydrogeology of the unsaturated zone, North Ramp area of the Exploratory Studies Facility, Yucca Mountain, U. S. Geological Survey, Water-Resources Investigation Report, Denver, CO, 1996 (draft).
- Soeder, D., Personal communication, 1995
- Wu, Y.S., S. Finsterle, P. Prefer, C.F. Ahlers, and A. Simmons, Softer qualification for ITOUGH2 and various equation-of-state (EOS) modules and auxiliary modules for TOUGH2 and ITOUGH2, Report LBL-xxxx, Lawrence Berkeley National Laboratory, Berkeley, CA (draft).
- Yang, I.C., Rattray, G.W., and P. Yu, Interpretations of chemical and isotopic data from boreholes in the unsaturated-zone at Yucca Mountain, Nevada, U. S. Geological Survey, Water-Resources Investigation Report-96-4058, Denver, CO, 1996.

THREE-DIMENSIONAL MODEL CALIBRATION AND SENSITIVITY STUDIES

Y.S. Wu, G. Chen, C. Haukwa, and G.S. Bodvarsson

August 1996

8.1 Introduction

The objective of this Chapter is to provide a comprehensive summary of the 3-D model calibration and sensitivity analysis, as part of our continuous efforts in the development of the three-dimensional unsaturated-zone site-scale model of Yucca Mountain during the fiscal year of 1996. The primary objectives of development of the 3-D site-scale unsaturated-zone model of Yucca Mountain are to develop a reliable and defensible computer model to simulate and investigate the existing natural state of the system, and predict possible future system responses. In order to provide accurate predictions of the mountain conditions, the site-scale model must include the following capabilities:

- Estimate the ambient and future moisture, gas and heat distributions and movement at Yucca Mountain;
- Estimate the percolation fluxes at repository horizons and their spatial and temporal variations;
- Provide a "best" set of hydrogeologic and thermal parameters for Performance Assessment (PA) calculations;
- Evaluate different conceptual models for hydrologic, pneumatic and heat flow;
- Evaluate effects of future climatic changes; and
- Evaluate effects of thermal loading.

As a critical step of model development, a series of model calibrations and sensitivity analyses has been conducted with the 3-D site-scale model this year. The model has been calibrated against available field observation and laboratory data. The sensitivity analyses are used to investigate effects of variations in rock and fault properties, and in model boundary conditions and various issues regarding conceptual models. The purpose of these model calibrations and sensitivity analyses is to enhance the accuracy and to increase the credibility of the site-scale model in estimating the current and predicting future conditions. Also these studies are necessary to provide critical data and information for total system performance analysis (TSPA) of the repository.

A substantial amount of model calibration has been performed so far (Ahlers et al., 1995a and b). However, in-depth model calibration studies are still needed as more field data become available and new observation data from the ESF are generated. The model calibration efforts reported in this chapter use saturation and moisture tension data, gas flow data, geothermal conditions and heat flow data, perched water data, and environmental isotope data. The environmental isotope data include isotopic concentrations in liquid and gas phases, as well as isotopes measured in fracture coatings which provide age estimates. The uncertainties associated with the input data set and the results of the model calibrations are also evaluated.

The TOUGH2 code (Pruess 1991) was used and the data on the perched water ages was used (Rousseau et al., 1996; Yang et al., 1996) to calibrate the site-scale model against the observation data of moisture and water potentials from 7 boreholes (USW UZ-14, UE-25 UZ-16, USW NRG-6, USW NRG-7a, USW SD-7, USW SD-9, and USW SD-12). We have developed several three-dimensional models which incorporate the observed moisture and geothermal data. All these models are based on the current 3-D site-scale model grid. In these simulations, both the generalized effective continuum method (ECM) (Chapter 4, Wu et al.) and dual-permeability model have been used to account for fracture and matrix interactions.

Many model simulations have been performed to quantify the sensitivity of the model to the parameters and assumptions that were used in the model preparations. The results of these studies will be used to provide direction for future modeling work and field data collection efforts in order to reduce uncertainties in future modeling studies. The sensitivity studies related to model set-up and input parameters include: infiltration rates, rock parameter studies, fracture/matrix flow, boundary conditions, and fault representations.

Additional sensitivity studies have also been performed to assess the effects of the chosen numerical modeling approaches used to handle fracture/matrix interactions in welded and unwelded tuffs of the unsaturated zone. Comparison studies have been done of the treatment of fracture/matrix flow using the generalized ECM approach, as discussed in Chapter 4 (Wu et al.), and the dual-permeability approach (Pruess, 1991). The comparative studies are conducted using the full site-scale model grid under the same model conditions. The results of the model predictions from the two modeling approaches are compared in terms of moisture distributions and movement within the mountain, and it has been shown that the ECM approach gives almost identical simulation results, when compared with the predictions by the dual-permeability model, under the modeling conditions and conceptual model used.

Three different infiltration maps have been incorporated into the UZ site-scale model. The first one uses a uniform infiltration rate of 0.1 mm/yr over the entire mountain, and this case is intended to form a basis for comparisons. The

second one is a spatially distributed infiltration map from USGS (Hevesi and Flint, 1995) with an averaged infiltration value of 0.34 mm/yr over the model domain. The third map is the most recent (Flint, Hevesi, and Flint, 1996), and has a much higher average infiltration rate of 4.4 mm/yr over the model area.

The rock properties for fractures and matrix used in modeling studies in each geological unit are those estimated using the ITOUGH2 code, and the detailed procedures for parameter estimation are described in Chapter 3 (Bandurraga et al.). The inverse modeling studies using ITOUGH2 (Chapter 3) result in several different sets of rock properties, which depend on the initial input to the code, the quality of the observed measurements, and the infiltration conditions. As part of sensitivity studies, four different sets of rock properties are implemented and tested in the simulations to investigate effects of rock properties variations and heterogeneity.

Even though substantial progress was made in the site characterization studies of Yucca Mountain over the past few years (Wittwer et al., 1995; Ahlers et al., 1995a and b; and Rousseau et al., 1996), many uncertainties still remain with regard to properties and roles of fault zones in affecting moisture flow through the mountain. In an effort to better understand the roles played by the major faults, we have conducted a series of sensitivity studies of fault properties on lateral and vertical moisture movement. The fault properties tested are derived from the pneumatic data analysis, and inverse model analysis results for the corresponding geological formations, as well as assumed values.

In all the simulations conducted for 3-D model calibrations and sensitivity analyses, the model predicted moisture distributions match well with observed water saturation profiles, and are in reasonable agreement with observed water potential or capillary pressure data from the 7 boreholes. The heat flow through the unsaturated zone simulated by the models is also in reasonable match with field measurements. By analyzing the computed downward flow through fractures and matrix rock, we are also able to match the water age data reasonably well at the areas near boreholes UZ-1/14 and SD-7.

Based on the confidence built through the model calibration and sensitivity analysis, we present simulation results and predictions on (1) lateral fluid movement through the mountain; (2) percolation flux at the repository horizon; (3) recharge maps at the water table, and (4) possible fast water flow pathways from surface to water table.

8.2 *QA Status of Data and Computer Software*

All the liquid saturation and water potential data from the seven boreholes UZ-14, UZ-16, NRG-6, NRG-7a, SD-7, SD-9, and SD-12 are "Q" data, and the data tracking references are listed in Table 8.2.1. These data have been used in

Three-Dimensional Model Calibration and Sensitivity Studies

this study for rock property estimation and also for 3-D model calibrations of moisture flow.

Table 8.2.1 Saturation and Capillary pressure Borehole Data from USGS (L. Flint, Principal Investigator)				
Borehole	Saturation	Capillary pressure	QA	Reference
SD-7	*	*	Y	YMP DTN GS951108312231.009
SD-9	*	*	Y	YMP DTN GS950308312231.004
SD-12	*		Y	YMP DTN GS950308312231.002
UZ-14	*	*	Y	YMP DTN GS950308312231.005
UZ#16	*		Y	YMP DTN GS940508312231.006
NRG-6	*		Y	YMP DTN GS950608312231.007
NRG-7a	*		Y	YMP DTN GS951108312231.010
where * denotes the data are available.				

The perched water zones are identified in five boreholes (UZ-1, UZ-14, SD-7, SD-9 and NRG-7a) in Yucca Mountain. The observations of depths, and relation to lithostratigraphy for perched water at UZ-14, SD-9, and NRG-7a are fully qualified (Rousseau et al., 1996). The perched water locations are used in the report to compare with the model results.

The temperature and heat flow data reported by Sass et al. (1988) were collected prior to implementation of the approved USGS-YMP quality-assurance program, and therefore are "non-Q". These temperature data are used in this study to generate model boundary conditions of temperature at the water table. The heat flow data are also employed to compare with model predictions. However, the surface temperature data from NRG-6 and NRG-7a are "Q" data.

The two infiltration maps used in this Chapter were from the two research reports of USGS (Hevesi and Flint, 1995; and Flint et al., 1996), which are in the process of being "Q'd" by the USGS.

The TOUGH2 code has been used as a primary computer tool in this simulation study, and it has been qualified (QA) for the YMP site characterization studies (Pruess et al., 1996). We also use one additional module, the ECM module of TOUGH2 as discussed in Chapter 3, which has been qualified for use in the YMP (Wu et al., 1996).

8.3 Model Description

8.3.1 Model Domain and Grid

The 3-D site-scale model domain and grid used in this study are shown in Figure 8.3.1 in a plan view. As shown in the figure, the model domain covers a total of surface area of approximate 37 km², extending roughly from borehole G-2, in the north, to borehole G-3, in the south, and from the Bow Ridge fault in the east to about one kilometer west of the Solitario Canyon fault. Figure 8.3.1 shows the numerical grid with increased discretization in the vicinity of the proposed repository. Also shown in Figure 8.3.1 are the locations of the seven boreholes which we will use for our model calibrations.

The model domain covered in the current site-scale model, as shown in Figure 8.3.1, was selected to focus our study at and near the potential repository area and to investigate effects of the major faults on moisture flow around the repository. All the model boundaries are located sufficiently far from the repository so that their effects on the simulation results at the repository are very small. The model domain may be need to be expanded in the future to the north to include the high water gradient effects.

The layering and subdivision of geological units in the numerical grid uses the geological model, discussed in detail in Chapter 2 (Bandurraga et al.). All grid layers have finite thicknesses across the model. The geological formation pinch-outs are represented by specifying the adjacent layer properties in the pinch-out locations. The site-scale model grid has 28 grid layers that represent different geological layers and altered zones in the unsaturated zone of Yucca Mountain. The top of the model is defined by subtracting the alluvium thickness from the topographical map. However, the alluvium unit is used in studies of pneumatic data (Ahlers et al., 1996). The Tiva Canyon unit (TCw) is vertically subdivided into three layers. Some layers are eroded and not present in certain locations. The Paintbrush unit (PTn) is represented using five grid layers with several layers pinching out in certain areas of the model. The Topopah Spring (TSw) uses seven sublayers and an additional three layers for the repository area. The Calico Hills (CHn) has a maximum of eight sublayers, but generally about five in most locations. The bottom boundary of the model is at the water table

Chapter 5 (Haukwa et al.) discusses the scheme and details on the grid generation. As shown in Figure 8.3.1, each grid layer has 983 element blocks, or the three-dimensional grid has 983 vertical grid columns. The total number of element blocks of the grid is 26,833, and the total connections between the blocks are 93,626.

Figure 8.3.1

A plan view of the 3-D site-scale model domain, grid and incorporated major faults.

Several major faults are incorporated explicitly in the model, as shown in Figure 8.3.1. These faults are Solitario Canyon, Iron Ridge, Ghost Dance, Abandoned Wash, and Dune Wash faults. The Bow Ridge fault is treated as a boundary condition along the eastern boundary of the model domain. The faults are represented in the model as vertical zones with consideration of stratigraphic offsets and connections to adjacent gridlayers. The scheme used for generating the fault grid elements was outlined by Wittwer et al. (1995) and also briefly discussed in Chapter 5 (Haukwa et al.).

8.3.2 Modeling Approach

The simulation results presented here were conducted using the TOUGH2 code (Pruess, 1991). Model calibrations, sensitivity analyses and model predictions mostly utilize the steady-state simulations of the 3-D models, under given infiltration rates and other boundary conditions. In addition, transient 3-D simulations were also performed to look at a possible climate change scenario using higher infiltration rates. The numerical modeling approaches for treatment of fracture/matrix flow include both the generalized ECM method (Chapter 4, Wu et al.) and the more rigorous dual-permeability approach. The formulation for the generalized ECM is discussed in Chapter 3 (Wu et al.) for treatment of fracture/matrix flow. In most of the simulation results presented

in this Chapter, the ECM model is used. However, the dual-permeability (dual-k) method was employed to investigate the effects of higher infiltration rates in terms of a possible climate change using the entire site-scale model grid.

It has been a long-debated issue whether the ECM approximation is valid and accurate for use in the site characterization studies of Yucca Mountain. This is because in simulating fluid and heat flow in the fractured, welded tuffs of the Yucca Mountain site it is critical to evaluate fracture and matrix interactions under multi-phase, non-isothermal conditions. There are several methods that have been used for treatment of fracture and porous matrix interactions using a numerical model. These methods include: (1) explicit discrete fracture and matrix treatment; (2) the effective-continuum model approach (ECM); (3) the double- or multiple-porosity method; (4) the dual-permeability method; and (5) more generally, the multiple interacting continua (MINC) method (Pruess and Narasimhan, 1985). The TOUGH2 code provides all these options for modeling fracture/matrix flow. When applied to simulating moisture flow and heat transfer at the mountain, all these approaches require knowledge of fracture and matrix properties and their spatial distribution. These site-specific fracture/matrix parameters, however, are presently not well defined for the tuffs at Yucca Mountain. Currently, only the effective-continuum approach has found wide application because of its simplicity in terms of data requirements and computational intensity.

As implemented in the site-scale model with the TOUGH2 code (See Chapter 4, Wu et al.), the ECM can accommodate two-phase flow in a fracture/matrix system. When applicable, the ECM provides a substantial simplification in description of fluid and heat flow in fractured porous media, and in the requirement of extensive computational efforts. The favorable conditions for this method is when rock matrix blocks are relatively small and permeable, and the fracture network is relatively uniformly distributed. However, the effective-continuum approximation may break down under certain unfavorable conditions, such as for very tight, large, and low permeability rock matrix blocks with rapid transients through surrounding fractures, since it may take a long time to reach equilibrium conditions under such environments.

At Yucca Mountain, the averaged net water infiltration rate into the unsaturated zone has been estimated to be low, on the order of 1 mm /yr. At most, the highest infiltration rates may be up to 10 mm/yr, as suggested by recent studies in certain areas of the mountain (Hudson and Flint, 1995; and Flint, Hevesi and Flint, 1996, in prep.). The percolation flux of water through the mountain is expected to be small in most locations. Therefore, the local hydraulic equilibrium between porous rock matrix and fractures may be a reasonable approximation, when one is interested in the ambient flow conditions. As a result, the ECM may provide reasonable simulation results for predicting the fluid movement and the ambient hydrogeologic conditions. The ECM will be particularly suitable for a situation when a long-term, averaged, or steady-state

solution is to be sought. As concluded by Pruess et al. (1990a,b), the effective-continuum approximation will be applicable when "sufficiently" large space and time scales are considered. Both time and space discretizations in the three-dimensional site-scale unsaturated-zone model are relatively large, and the application of the continuum approach may be justified for time and space scales of interest to the site-scale modeling studies. Issues regarding the proper use of the various numerical approaches including ECM, dual-permeability, dual-porosity and others are evaluated for various processes in Chapter 6 (Doughty et al.).

The water ages determined from isotope data, perched water samples, fracture coatings, and water travel modeling results suggest that the water currently found at Yucca Mountain has been in the subsurface for thousands of years. Under such a large time scale, the ambient moisture flow and distributions at Yucca Mountain can be reasonably approximated using steady-state or near steady-state conditions. This is the reason that we mainly use steady-state simulations in the model calibration and sensitivity analysis studies of this chapter. Another reason is the fact that model results are dependent on poorly constrained transient infiltration events, and it is difficult to decide which transient infiltration conditions should be used to compare with the observed data.

8.3.3 Model Boundary Conditions

The ground surface of the mountain or bottom of the alluvium is taken as the top model boundary, and the water table is treated as the bottom boundary. Both top and bottom boundaries of the model are treated as Dirichlet-type conditions, i.e., constant (but distributed) temperatures, constant (but distributed) gas pressures and constant liquid saturations are specified along the boundary surfaces. In addition to the pressure and temperature conditions, the surface boundary is also subject to water recharge through infiltration, as discussed in the next section.

The constant values of temperatures on the boundaries are determined based on the field observations. For the bottom temperatures at the water table, the temperature values specified were taken and interpolated from the borehole temperature measurement data, reported by Sass et al. (1988). The results of temperature distributions, as implemented in the model, are shown in Figure 8.3.2. The temperature values at the water table are generally higher in the southern part, and lower in the northern part of the model domain. The highest temperatures are near the south-west corner, and the lowest are in the north, close to borehole G-2. The temperature map of the water table is consistent with that of Fridrich et al. (1994), with an averaged value of about 32°C.

Figure 8.3.2
Temperature map at the water table for the bottom temperature boundary condition of the 3-D site-scale model.

To account for differences in temperature on the mountain at different elevations, we use both observed wellhead temperature data and the equation which correlates temperature with elevation. The surface temperatures are estimated using observed temperature data from boreholes USW NRG-6 and NRG-7a, which have more than a year of continuous temperature monitoring data (Rousseau et al., 1996). The following formulation (Lu and Kwicklis, 1995) is also used,

$$T_a = T_{ref} + \lambda(Z_{ref} - Z) \quad (8.3.3.1)$$

where T_a is ground surface temperature at elevation Z , T_{ref} is temperature at reference elevation Z_{ref} , and λ is atmospheric lapse rate ($^{\circ}\text{C}/\text{m}$).

The annually averaged temperature at NRG-6 is 18.23 $^{\circ}\text{C}$, and at NRG-7a, it is 17.78 $^{\circ}\text{C}$ (Rousseau et al., 1996). Using the surface elevation data and the annually averaged temperatures at the two boreholes, we can calculate the atmospheric lapse rate, $\lambda \approx 0.01$ $^{\circ}\text{C}/\text{m}$ at Yucca Mountain. Then the surface temperatures are determined using Equation (8.3.3.1) and elevations of the top model meshes. The resulting surface temperature distributions are shown in

Figure 8.3.3. The figure shows that there are relatively lower temperatures in the northern part and along the ridge of the mountain, where higher elevations exist, and the temperatures are at the lower teens in °C. In the rest of the model domain, Figure 8.3.3 indicates an average temperature of 16 - 18 °C.

Figure 8.3.3
Temperature map on the ground surface for the top temperature boundary condition of the 3-D site-scale model.

The gas pressures at the bottom boundaries are calculated using the observed gas pressure value (Ahlers et al., 1995a). The water table, as the bottom boundary of the site-scale model, is a relatively flat, stable surface. The water table, in the eastern part to the Solitario Canyon fault, has an approximate elevation of 730 m. However, the water table rises 40 meters across the Solitario Canyon fault to the west. The gas pressures are estimated using a pressure value of 0.92 bars at an elevation of 730 m. All the gas pressures of the bottom boundary elements are then calculated using elevations relative to the 730 m elevation for each boundary grid block, assuming that hydrostatic conditions exist. The water table treatment in this Chapter follows mostly the work of Wittwer et al. (1995), and the apparent high potentiometric surface in the north of the model boundary is not considered.

Surface gas pressures are determined by running TOUGH2 to steady-state conditions under given temperature, bottom pressure, and surface infiltration conditions. This is necessary to generate a steady-state, equilibrated gas pres-

sure boundary to avoid artificial air flow or circulation, which may happen when non-equilibrated pressures are imposed on the ground surface boundaries.

All the lateral boundaries, as shown in Figure 8.3.1, are treated as no-flow, or closed boundaries, which are default options for the TOUGH2 code. This treatment should be reasonable for the eastern boundary, which is along the Bow Ridge fault, since high vertical permeability and lower capillary forces are expected for the fault. For the southern, western, and northern, lateral boundaries, no-flow boundaries may have little effects on moisture flow within and near the potential repository areas, since these boundaries are far away from the repository.

8.4 *Implementation of Different Infiltration Maps*

Infiltration, or net water infiltration, through the top soil layer of the mountain is the most significant factor affecting the overall hydrological and thermohydrologic behavior of the unsaturated zone. The net infiltration is the ultimate source of groundwater recharge and percolation through the unsaturated zone, and provides the water for flow and transport mechanisms for radionuclides from repository to water table. Net infiltration at Yucca Mountain is highly variable spatially because there exist significant variations in soil cover and different mechanisms controlling the net infiltration from the precipitation (Flint and Flint, 1994, Hudson and Flint, 1995). Even though substantial research efforts have been made in the past to determine the net infiltration over the mountain, direct measurements have proven impossible due to the low moisture flux resulting from the low precipitation and high potential evapotranspiration rates of the area.

Most of the effort on estimating the net infiltration at the site has been based on the average annual precipitation using an indirect method, with results ranging between 0 to more than 20 mm/yr. The spatial variability of net infiltration at the site estimated by Flint and Flint (1994) ranged from 0.02 to 13.40 mm/yr. Their estimation was based on hydraulic property measurements of the bedrock units close to the surface, the steady state water content, and an assumed unit gradient. In 1995, their work was extended to develop a map to describe the spatial distribution of shallow infiltration at Yucca Mountain (Hudson and Flint, 1995). This study, based on the neutron moisture meter data from 84 locations conducted over ten years and a multiple linear regression model, gave a much higher net infiltration over a modeled area of 150 km², with an average of 21.6 mm/yr.

A recent study for estimating precipitation and recharge in the Yucca mountain region by Hevesi and Flint (1995) provided another infiltration map, which gives an averaged value of 0.35 mm/yr net infiltration over the site-scale model

domain. The infiltration map was generated using the geostatistical Maxey-Eakin model. Figure 8.4.1 shows the distribution of net water infiltration over the model domain from this infiltration map. High infiltration rates are noticed at the northern part of the model domain and along the south-north ridge of the mountain. Much lower infiltration can be seen along or near the Bow Ridge fault, the eastern part, and near the south-west corner of the model area. This infiltration map has been implemented and used in our model calibration and sensitivity analysis studies, and it is referred as to Map #1 in this Chapter.

The most recent infiltration map has been recently supplied to us from the USGS (Flint, Hevesi and Flint, July, 1996). This new map is also used for the modeling studies in this report. Figure 8.4.2 shows how the net infiltration is distributed over the site-scale model domain. The averaged infiltration rate is 4.4 mm/yr, which is more than ten times higher than that shown in Figure 8.4.1. However, the spatial distributions of infiltration, in Figure 8.4.2, are very similar to that in Figure 8.4.1, with higher recharge values in the north part of the model domain and along the mountain ridge from south to north. This infiltration is referred as to Map # 2 in this study.

Figure 8.4.1

Net infiltration map (Map # 1) showing infiltration rates and distributions over the model domain of Yucca Mountain, based on Maxey-Eakin model (Hevesi and Flint, Nov., 1995).

Figure 8.4.2

Net infiltration map (Map # 2) showing infiltration rates and distributions over the model domain of Yucca Mountain (Flint, Hevesi and Flint, July, 1996).

In addition to the two infiltration maps from the USGS, we also use uniform infiltration rates, such as 0.1 mm/yr, in our sensitivity studies. The uniform infiltration rates are simpler to implement, and still can give us many insights into the effects of parameter variations. Also, use of uniform infiltration rates has resulted in a good match with the observed saturation and water potential data in many cases.

While there exists a high degree of uncertainty with regard to the steady-state net infiltration rates over the mountain, the past and future climate variations and their impacts on net infiltration are even more uncertain. We have tried to address the issue of climatic changes by using a much higher infiltration rate (actually 3 times) to cover the worst case scenarios. The high infiltration rates used are a step-change from the infiltration map # 2 (Figure 8.4.2), which follows the steady-state ambient condition based on the infiltration map # 2.

8.5 Model Parameters and Rock Properties

All the simulations presented in this Chapter were performed using the TOUGH2 code (Pruess, 1991). Thermophysical properties of liquid water and vapor in the TOUGH2 code are internally generated within experimental accuracy from steam table equations (International Formulation Committee, 1967).

Air is treated as an ideal gas and additivity of partial pressures is assumed for air/vapor mixtures.

The rock thermal conductivities and rock thermal capacities used are from Reference Information Base (RIB) (DOE, 1993) for the Yucca Mountain tuffs. The detailed discussion regarding the rock thermal properties is given in Chapter 9 (Bodvarsson et al.) of this report.

The rock properties used for matrix and fracture were estimated using the ITOUGH2 code (Finsterle, 1993), based on the QA saturation and water potential data as initial estimates. The methodology and procedure of the parameter estimation is presented in Chapter 3 (Bandurraga et al.). In the parameter estimation studies of Chapter 3, different infiltration rates, and initial estimates of parameters were used. Therefore, several sets of rock properties have been obtained, depending on the inverse model input specification and conceptual models. Four sets of the rock properties estimated in Chapter 3 have been used in this chapter for model calibration and sensitivity studies, as discussed below.

The rock parameter specification in the 3-D site-scale model is, in general, layer-wise, but some zones located in certain grid layers in the CHn unit are zeolitic regions. In these layers zeolitic and vitric tuff properties will be specified for corresponding geologic zones and locations. The whole unsaturated-zone formation system is subdivided, in general, into 28 hydrogeological units or gridlayers, as discussed in Chapter 2 (Bandurraga). We treat all of the geological units as fracture/matrix systems, except for the PTn unit, which is treated as a single continuum porous medium. This approach will be investigated in UZ modeling studies in FY 1997.

The tables for rock properties used are given in the following, and we also list bulk porosities for matrix and fracture rock. These porosity values were not estimated by our inverse model studies. The matrix porosities were taken from the USGS data (Flint, 1996, in prep.), and fracture porosities were from the GWTT-95 report (Ho et al., 1995).

8.5.1 Parameter Set # 1

The rock properties, parameter set #1, are considered the base-case parameter set. This set of parameters was estimated using a uniform infiltration rate of 0.1 mm/yr, and observations from five boreholes (Chapter 3). The initial estimates of parameters were based on the most updated rock properties from USGS (Flint, 1996, in prep.). The properties for matrix and fracture rock for parameter set #1 are listed in Table 8.5.1. The units in the table for the hydrogeologic units or grid layers are discussed in Chapter 2 (Bandurraga et al.) and later in this section.

Three-Dimensional Model Calibration and Sensitivity Studies

Table 8.5.1
The rock properties, parameter set #1, of matrix and fractures used in the model calibration and sensitivity studies.

Units	k_m (m ²)	k_f (m ²)	α_m (Pa ⁻¹)	α_f (Pa ⁻¹)	m_m	m_f	ϕ_m	ϕ_f
tcw11	0.160E-18	0.601E-11	0.188E-04	0.155E-02	0.229	0.227	0.062	0.290E-03
tcw12	0.340E-16	0.575E-11	0.131E-05	0.123E-02	0.232	0.231	0.082	0.290E-03
tcw13	0.219E-16	0.575E-11	0.135E-05	0.123E-02	0.461	0.437	0.207	0.290E-03
ptn21	0.399E-12	n/a	0.219E-04	n/a	0.219	n/a	0.435	n/a
ptn22	0.239E-12	n/a	0.119E-04	n/a	0.310	n/a	0.222	n/a
ptn23	0.755E-14	n/a	0.365E-04	n/a	0.235	n/a	0.406	n/a
ptn24	0.880E-13	n/a	0.304E-04	n/a	0.289	n/a	0.499	n/a
ptn25	0.310E-12	n/a	0.183E-03	n/a	0.224	n/a	0.490	n/a
tsw31	0.253E-14	0.399E-11	0.257E-04	0.136E-02	0.205	0.203	0.048	0.243E-03
tsw32	0.676E-14	0.100E-10	0.181E-04	0.863E-03	0.248	0.250	0.156	0.243E-03
tsw33	0.214E-17	0.629E-11	0.659E-05	0.544E-03	0.248	0.268	0.154	0.243E-03
tsw34	0.252E-16	0.399E-11	0.801E-06	0.121E-02	0.321	0.320	0.110	0.243E-03
tsw35	0.334E-16	0.399E-11	0.350E-05	0.121E-02	0.224	0.227	0.130	0.243E-03
tsw36	0.959E-16	0.399E-11	0.561E-06	0.121E-02	0.414	0.416	0.112	0.243E-03
tsw37	0.200E-16	0.399E-11	0.112E-05	0.121E-02	0.370	0.368	0.036	0.243E-03
ch1vc	0.160E-11	0.723E-12	0.895E-04	0.121E-02	0.224	0.227	0.273	0.111E-03
ch2vc	0.218E-13	0.723E-12	0.716E-04	0.121E-02	0.219	0.227	0.344	0.111E-03
ch3vc	0.218E-13	0.723E-12	0.716E-04	0.121E-02	0.219	0.227	0.344	0.111E-03
ch4vc	0.218E-13	0.723E-12	0.716E-04	0.121E-02	0.219	0.227	0.344	0.111E-03
ch1zc	0.539E-15	0.100E-12	0.189E-06	0.729E-03	0.356	0.359	0.288	0.525E-04
ch2zc	0.713E-18	0.100E-12	0.518E-05	0.729E-03	0.225	0.225	0.332	0.525E-04
ch3zc	0.713E-18	0.100E-12	0.518E-05	0.729E-03	0.225	0.225	0.332	0.525E-04
ch4zc	0.840E-17	0.100E-12	0.150E-06	0.729E-03	0.475	0.476	0.266	0.525E-04
pp3vp	0.521E-15	0.299E-13	0.206E-04	0.121E-02	0.306	0.313	0.322	0.111E-03
pp2zp	0.170E-16	0.100E-12	0.179E-05	0.729E-03	0.311	0.312	0.286	0.525E-04
bf3vb	0.521E-15	0.299E-13	0.206E-04	0.121E-02	0.306	0.313	0.322	0.111E-03
bf2zb	0.170E-16	0.100E-12	0.179E-05	0.729E-03	0.311	0.312	0.286	0.525E-04
tm3vt	0.521E-15	0.299E-13	0.206E-04	0.121E-02	0.306	0.313	0.322	0.111E-03

In table 5.5.1 and the following tables, k_m and k_f are saturated matrix and fracture continuum permeabilities; α_m and α_f are van Genuchten's parameter of capillary pressure of matrix and fracture; m_m and m_f are van Genuchten's parameter of soil retention curves; and ϕ_m and ϕ_f are porosities of matrix and fracture systems, respectively.

Three-Dimensional Model Calibration and Sensitivity Studies

8.5.2

Parameter Set # 2

The rock properties, parameter set #2, were estimated using a uniform infiltration rate as in set #1, and data from five boreholes. But the initial estimates of parameters, as the input to the ITOUGH2 code, were based on the previous rock properties from USGS, L. Flint (see sensitivity studies, Chapter 3, Bandurraga et al.). The properties for matrix and fracture rock for parameter set #2 are listed in Table 8.5.2.

Table 8.5.2
The rock properties, parameter set #2, of matrix and fractures used in the model calibration and sensitivity studies.

Units	k_m (m ²)	k_f (m ²)	α_m (Pa ⁻¹)	α_f (Pa ⁻¹)	m_m	m_f	ϕ_m	ϕ_f
tcw11	0.179E-19	0.519E-11	0.351E-05	0.235E-03	0.414	0.585	0.062	0.290E-03
tcw12	0.104E-15	0.576E-11	0.226E-05	0.596E-03	0.486	0.412	0.082	0.290E-03
tcw13	0.116E-17	0.621E-11	0.351E-05	0.776E-04	0.545	0.501	0.207	0.290E-03
ptn21	0.181E-14	n/a	0.253E-04	n/a	0.206	n/a	0.435	n/a
ptn22	0.504E-14	n/a	0.150E-04	n/a	0.138	n/a	0.222	n/a
ptn23	0.126E-13	n/a	0.200E-04	n/a	0.240	n/a	0.406	n/a
ptn24	0.126E-13	n/a	0.286E-04	n/a	0.344	n/a	0.499	n/a
ptn25	0.362E-14	n/a	0.376E-04	n/a	0.263	n/a	0.490	n/a
tsw31	0.385E-16	0.249E-11	0.125E-04	0.306E-03	0.368	0.294	0.048	0.243E-03
tsw32	0.276E-16	0.962E-11	0.751E-05	0.611E-04	0.243	0.254	0.156	0.243E-03
tsw33	0.636E-18	0.483E-11	0.251E-05	0.110E-03	0.333	0.418	0.154	0.243E-03
tsw34	0.359E-17	0.479E-11	0.667E-06	0.876E-04	0.552	0.459	0.110	0.243E-03
tsw35	0.179E-18	0.497E-11	0.173E-05	0.921E-04	0.289	0.419	0.130	0.243E-03
tsw36	0.322E-18	0.457E-11	0.592E-06	0.611E-04	0.387	0.399	0.112	0.243E-03
tsw37	0.669E-16	0.409E-11	0.735E-06	0.114E-03	0.464	0.438	0.036	0.243E-03
ch1vc	0.602E-11	0.723E-12	0.157E-05	0.240E-03	0.469	0.518	0.273	0.111E-03
ch2vc	0.199E-11	0.723E-12	0.320E-05	0.240E-03	0.554	0.742	0.344	0.111E-03
ch3vc	0.199E-11	0.723E-12	0.320E-05	0.240E-03	0.554	0.742	0.344	0.111E-03
ch4vc	0.199E-11	0.723E-12	0.320E-05	0.240E-03	0.554	0.742	0.344	0.111E-03
ch1zc	0.114E-14	0.100E-12	0.251E-06	0.735E-04	0.505	0.518	0.288	0.525E-04
ch2zc	0.266E-17	0.560E-13	0.547E-06	0.755E-04	0.319	0.321	0.332	0.525E-04
ch3zc	0.266E-17	0.560E-13	0.547E-06	0.755E-04	0.319	0.321	0.332	0.525E-04
ch4zc	0.741E-20	0.121E-12	0.103E-05	0.365E-04	0.489	0.639	0.266	0.525E-04
pp3vp	0.279E-11	0.300E-13	0.900E-05	0.133E-03	0.363	0.467	0.322	0.111E-03
pp2zp	0.956E-16	0.654E-13	0.823E-05	0.372E-03	0.213	0.206	0.286	0.525E-04
bf3vb	0.279E-11	0.300E-13	0.900E-05	0.133E-03	0.363	0.467	0.322	0.111E-03
bf2zb	0.956E-16	0.654E-13	0.823E-05	0.372E-03	0.213	0.206	0.286	0.525E-04
tm3vt	0.279E-11	0.300E-13	0.900E-05	0.133E-03	0.363	0.467	0.322	0.111E-03

Three-Dimensional Model Calibration and Sensitivity Studies

8.5.3

Parameter Set # 3

The rock properties, parameter set #3, was estimated using the infiltration map #1 (Figure 8.4.1), and data from five boreholes. The initial estimates of parameters, the same as those used for parameter set # 1, based on the updated rock properties from USGS (Flint, 1996). The properties for matrix and fracture rock for parameter set #3 are listed in Table 8.5.3.

Table 8.5.3 The rock properties, parameter set #3, of matrix and fractures used in the model calibration and sensitivity studies.								
Units	k_m (m^2)	k_f (m^2)	α_m (Pa^{-1})	α_f (Pa^{-1})	m_m	m_f	ϕ_m	ϕ_f
tcw11	0.821E-19	0.118E-10	0.104E-04	0.231E-03	0.497	0.575	0.062	0.290E-03
tcw12	0.406E-15	0.592E-11	0.219E-05	0.150E-02	0.523	0.411	0.082	0.290E-03
tcw13	0.191E-16	0.599E-11	0.384E-05	0.113E-02	0.501	0.516	0.207	0.290E-03
ptn21	0.303E-15	n/a	0.744E-04	n/a	0.219	n/a	0.435	n/a
ptn22	0.837E-12	n/a	0.119E-04	n/a	0.309	n/a	0.222	n/a
ptn23	0.134E-14	n/a	0.100E-03	n/a	0.352	n/a	0.406	n/a
ptn24	0.789E-14	n/a	0.123E-04	n/a	0.406	n/a	0.499	n/a
ptn25	0.123E-13	n/a	0.221E-03	n/a	0.289	n/a	0.490	n/a
tsw31	0.602E-16	0.723E-11	0.129E-04	0.432E-03	0.260	0.246	0.048	0.243E-03
tsw32	0.281E-16	0.125E-10	0.267E-04	0.109E-03	0.191	0.304	0.156	0.243E-03
tsw33	0.953E-18	0.168E-10	0.222E-05	0.139E-03	0.352	0.404	0.154	0.243E-03
tsw34	0.349E-18	0.440E-10	0.605E-06	0.496E-04	0.444	0.460	0.110	0.243E-03
tsw35	0.882E-19	0.967E-10	0.113E-05	0.105E-03	0.351	0.454	0.130	0.243E-03
tsw36	0.124E-16	0.436E-11	0.472E-06	0.111E-02	0.397	0.387	0.112	0.243E-03
tsw37	0.595E-16	0.419E-11	0.667E-06	0.112E-02	0.399	0.439	0.036	0.243E-03
ch1vc	0.787E-11	0.751E-12	0.949E-06	0.155E-02	0.469	0.517	0.273	0.111E-03
ch2vc	0.396E-11	0.660E-12	0.284E-05	0.133E-02	0.602	0.742	0.344	0.111E-03
ch3vc	0.396E-11	0.660E-12	0.284E-05	0.133E-02	0.602	0.742	0.344	0.111E-03
ch4vc	0.396E-11	0.660E-12	0.284E-05	0.133E-02	0.602	0.742	0.344	0.111E-03
ch1zc	0.117E-14	0.101E-12	0.876E-06	0.724E-03	0.469	0.518	0.288	0.525E-04
ch2zc	0.428E-17	0.617E-13	0.431E-06	0.628E-03	0.334	0.320	0.332	0.525E-04
ch3zc	0.428E-17	0.617E-13	0.431E-06	0.628E-03	0.334	0.320	0.332	0.525E-04
ch4zc	0.871E-20	0.210E-12	0.129E-05	0.384E-04	0.519	0.592	0.266	0.525E-04
pp3vp	0.126E-11	0.325E-13	0.472E-04	0.144E-02	0.196	0.466	0.322	0.111E-03
pp2zp	0.513E-15	0.100E-12	0.166E-05	0.660E-03	0.228	0.206	0.286	0.525E-04
bf3vb	0.126E-11	0.325E-13	0.472E-04	0.144E-02	0.196	0.466	0.322	0.111E-03
bf2zb	0.513E-15	0.100E-12	0.166E-05	0.660E-03	0.228	0.206	0.286	0.525E-04
tm3vt	0.126E-11	0.325E-13	0.472E-04	0.144E-02	0.196	0.466	0.322	0.111E-03

Three-Dimensional Model Calibration and Sensitivity Studies

8.5.4

Parameter Set # 4

The rock properties, parameter set #4, were estimated using the infiltration map # 2, and data from five boreholes. The initial estimates of parameters, the same as those used for parameter set # 1, are based on the updated rock properties from USGS (Flint, 1996). The properties for matrix and fracture rock for parameter set #4 are listed in Table 8.5.4.

Table 8.5.4 The rock properties, parameter set #4, of matrix and fractures used in the model calibration and sensitivity studies.								
Units	k_m (m^2)	k_f (m^2)	α_m (Pa^{-1})	α_f (Pa^{-1})	m_m	m_f	ϕ_m	ϕ_f
tcw11	0.160E-18	0.910E-11	0.147E-04	0.518E-03	0.238	0.182	0.062	0.290E-03
tcw12	0.540E-15	0.575E-11	0.174E-05	0.977E-03	0.233	0.223	0.082	0.290E-03
tcw13	0.220E-16	0.575E-11	0.129E-05	0.123E-02	0.463	0.437	0.207	0.290E-03
ptn21	0.400E-12	n/a	0.244E-04	n/a	0.215	n/a	0.435	n/a
ptn22	0.240E-12	n/a	0.159E-04	n/a	0.310	n/a	0.222	n/a
ptn23	0.111E-12	n/a	0.445E-04	n/a	0.243	n/a	0.406	n/a
ptn24	0.880E-13	n/a	0.341E-04	n/a	0.295	n/a	0.499	n/a
ptn25	0.105E-11	n/a	0.138E-03	n/a	0.243	n/a	0.490	n/a
tsw31	0.261E-12	0.400E-11	0.237E-04	0.122E-02	0.206	0.203	0.048	0.243E-03
tsw32	0.194E-12	0.445E-11	0.172E-04	0.969E-03	0.248	0.249	0.156	0.243E-03
tsw33	0.796E-17	0.743E-11	0.573E-05	0.243E-03	0.247	0.250	0.154	0.243E-03
tsw34	0.100E-14	0.159E-11	0.754E-06	0.686E-03	0.321	0.325	0.110	0.243E-03
tsw35	0.423E-15	0.400E-11	0.234E-05	0.108E-02	0.231	0.226	0.130	0.243E-03
tsw36	0.776E-16	0.400E-11	0.522E-06	0.122E-02	0.416	0.416	0.112	0.243E-03
tsw37	0.316E-15	0.400E-11	0.804E-06	0.122E-02	0.368	0.368	0.036	0.243E-03
ch1vc	0.160E-11	0.723E-12	0.760E-04	0.122E-02	0.221	0.227	0.273	0.111E-03
ch2vc	0.550E-13	0.723E-12	0.980E-04	0.122E-02	0.223	0.227	0.344	0.111E-03
ch3vc	0.550E-13	0.723E-12	0.980E-04	0.122E-02	0.223	0.227	0.344	0.111E-03
ch4vc	0.550E-13	0.723E-12	0.980E-04	0.122E-02	0.223	0.227	0.344	0.111E-03
ch1zc	0.540E-15	0.100E-12	0.190E-06	0.730E-03	0.359	0.359	0.288	0.525E-04
ch2zc	0.450E-17	0.100E-12	0.394E-05	0.388E-03	0.225	0.225	0.332	0.525E-04
ch3zc	0.450E-17	0.100E-12	0.394E-05	0.388E-03	0.225	0.225	0.332	0.525E-04
ch4zc	0.210E-16	0.100E-12	0.150E-06	0.730E-03	0.475	0.470	0.266	0.525E-04
pp3vp	0.542E-14	0.300E-13	0.194E-04	0.122E-02	0.316	0.313	0.322	0.111E-03
pp2zp	0.269E-15	0.100E-12	0.126E-05	0.730E-03	0.311	0.312	0.286	0.525E-04
bf3vb	0.542E-14	0.300E-13	0.194E-04	0.122E-02	0.316	0.313	0.322	0.111E-03
bf2zb	0.269E-15	0.100E-12	0.126E-05	0.730E-03	0.311	0.312	0.286	0.525E-04
tm3vt	0.542E-14	0.300E-13	0.194E-04	0.122E-02	0.316	0.313	0.322	0.111E-03

Three-Dimensional Model Calibration and Sensitivity Studies

8.5.5

Rock Name and Specification

As can be seen in the first columns of Tables 8.5.1 - 8.5.4, we have used "ROCK NAMES" or geological units for different model layers. The convention used for naming the rock types in different model grid layers is defined in Table 8.5.5. Table 8.5.5 also lists the corresponding information and definition regarding geological and hydrogeological units, formations, and model grid layers.

Table 8.5.5				
The corresponding relations of rock names, geological and hydrogeological units, formation and model grid layers used in the site-scale model.				
Geological Unit	Welding Intensity/ Formation Name (Buesch et al., 1995)	Model Grid Layer Name	Hydrogeological Unit	
PAINTBRUSH GROUP				
Tiva Canyon	M,D ¹ (Tpcoxxx)	tcw11 tsw12	Tiva Canyon (TCw)	
Tuff	D- Basal Vitrophyre (Tpcpv3)			
	M (Tpcpv2)	tcw13		
	N,P (Tpcpv1)	ptn21	Paintbrush (PTn)	
Bedded tuff	N (Tpbt4)			
Yucca Mountain Tuff	N,P,M (Tpy)	ptn22		
Bedded tuff	N (Tpbt3)	ptn23		
Pah Canyon Tuff	N,P,M (Tpy)	ptn24		
Bedded tuff	N (Tpbt2)		Topopah Spring (TSw)	
Topopah Spring Tuff	N,P (Tpdrv3)	ptn25		
	M (Tpdrv2)	tsw31		
	D -Upper vitrophyre (Tpdrv1)			
	M,D (Tpdrn)	tsw32		
	M,D,L (Tpdr1)			
	M,D,L (Tpdpul)	tsw33		
	D (Tpdrpmn)	tsw34		
	M,D,L (Tpdp11)	tsw35		
	D (Tpdrpln)	tsw36		
	D (Tpdrpv3)	tsw37		
Bedded tuff	N,P,M; may be altered (Tpdrpv1, Tpdrpv2)		Calico Hills (CHn)	
	N; may be altered (Tpdr1)	ch1zc, ch1vc		
Calico Hills Formation	N; unaltered (Ta - Vitric)	ch2vc		
	N; altered (Ta - Zeolitic)	ch3zc		
	N; may be altered (Tabt1)	ch4zc, ch4vc		
CRATER FLAT GROUP				

Three-Dimensional Model Calibration and Sensitivity Studies

Table 8.5.5 (cont.) The corresponding relations of rock names, geological and hydrogeological units, formation and model grid layers used in the site-scale model.			
Geological Unit	Welding Intensity/ Formation Name (Buesch et al., 1995)	Model Grid Layer Name	Hydrogeological Unit
Prow Pass Tuff	N; may be altered (Tpc) Unit 4 ³		
	N,P,M Unit 3	pp3vp	
	N,P; generally altered Units 2,1	pp2zp	
Bedded tuff	N; generally altered (Tpcbt1)		
Upper Bullfrog Tuff	N,P; generally altered (Tcb)		
Middle Bullfrog Tuff	N,P,M	bf3vp	Crater Flat Undifferentiated (CFu)
Lower Bullfrog Tuff	N,P; generally altered	bf2zp	
Bedded tuff	N; generally altered (Tcbbt)		
Upper Tram Tuff	N,P; generally altered (Tct)	tm3vt	

8.5.6 Fault Properties

Three sets of fault properties are used in this chapter to investigate effects of fault properties on moisture flow in the unsaturated zone of the mountain. The fault properties were based on the previous study (Wittwer et al., 1995; and Ahlers et al., 1995a), and the pneumatic data analysis at LBNL with USGS data (Ahlers et al., 1996). The major faults incorporated into the site-scale model are shown in Figure 8.3.1. Fault zones are treated as fracture/matrix media using the ECM approximation, instead of a single continuum porous medium, as specified in the previous study (Wittwer et al., 1995). The reason for using the ECM treatment is that fault zones consist of highly permeable fractures and matrix blocks with low permeability. However, the fracture system in faults has low porosity, or low storage capability for fluids. On the other hand, the matrix blocks are very low in permeability, but have large porosity, or more storage space. The ECM approach will include effects of both fractures and matrix in the fault zones.

The fault properties are based on our current understanding of the roles of faults, the pneumatic analysis, and the model calibrations. These are all considered to be Q data except for fault properties from Chapter 3.

The properties for Fault #1 are listed in Table 8.5.6, which shows that uniform fault properties are specified for all the incorporated faults in this case. A matrix permeability of 100 md is used for matrix blocks in faults, and horizontal and vertical permeabilities for fractures in faults are 10 and 100 darcies, respectively.

Three-Dimensional Model Calibration and Sensitivity Studies

Table 8.5.6 The rock properties for fault #1 used in the model calibration and sensitivity studies.									
Units	k_m (m ²)	$k_{f,h}$ (m ²)	$k_{f,v}$ (m ²)	α_m (Pa ⁻¹)	α_f (Pa ⁻¹)	m_m	m_f	ϕ_m	ϕ_f
All	1.00E-13	1.0E11	1.0-10	0.61E-4	0.61E-4	0.50	0.50	0.30	0.001

In Table 8.5.6, $k_{f,h}$ and $k_{f,v}$ are fracture permeabilities in horizontal and vertical directions, respectively, for the faults.

The second set of fault properties are provided in Table 8.5.7, and the only difference from the fault # 1 properties is that different continuum fracture permeabilities are used for fractures of the faults, which are subdivided into four geological units. The fracture permeability values are taken from the pneumatic data analysis of the fault permeability (Ahlers et al., 1996).

Table 8.5.7 The rock properties for fault #2 used in the model calibration and sensitivity studies.									
Units	k_m (m ²)	$k_{f,h}$ (m ²)	$k_{f,v}$ (m ²)	α_m (Pa ⁻¹)	α_f (Pa ⁻¹)	m_m	m_f	ϕ_m	ϕ_f
TCw	1.0E-13	2.0e-11	2.0e-11	0.61E-4	1.0e-3	0.50	0.50	0.30	0.001
PTn	1.0E-13	0.2e-12	0.2e-12	0.61E-4	1.0e-3	0.50	0.50	0.30	0.001
TSw	1.0E-13	2.0e-11	2.0e-11	0.61E-4	1.0e-3	0.50	0.50	0.30	0.001
CHn	1.0E-13	1.0e-14	1.0e-14	0.61E-4	1.0e-3	0.50	0.50	0.30	0.001

The third set of fault properties are given in Table 8.5.8. In this data set the two-phase flow parameters for relative permeability and capillary pressures are modified from those in Table 8.5.6 or Table 8.5.7. The van Genuchten parameters were changed using the selected values of parameter set # 4, as given in Table 8.5.4, for the matrix properties in the corresponding four fault units, respectively.

Table 8.5.8 The rock properties for fault #3 used in the model calibration and sensitivity studies.									
Units	k_m (m ²)	$k_{f,h}$ (m ²)	$k_{f,v}$ (m ²)	α_m (Pa ⁻¹)	α_f (Pa ⁻¹)	m_m	m_f	ϕ_m	ϕ_f
TCw	1.0E-13	2.0e-11	2.0e-11	0.18E-5	0.97e-3	.234	.223	0.30	0.001
PTn	1.0E-13	0.2e-12	0.2e-12	0.44E-4	1.00e-3	.243	.500	0.30	0.001
TSw	1.0E-13	2.0e-11	2.0e-11	0.24E-5	1.08e-2	.228	.226	0.30	0.001
CHn	1.0E-13	1.0e-14	1.0e-14	0.98E-4	1.00e-3	.223	.227	0.30	0.001

8.6 Comparisons with Observed Borehole Data

As a first step for model calibrations of the site-scale model, borehole measured saturation and water potential data are used to compare with the model predictions, based on different parameter sets. The liquid saturation and water potential data are from 7 boreholes UZ-14, UZ-16, NRG-6, NRG-7a, SD-7, SD-9, and SD-12, which were collected by the USGS (OCRWM, DOE, 1995). These data have been used in this study for analyzing effects of rock property variations and comparative studies between model simulations and observations. The locations of these 7 boreholes are shown in Figure 8.3.1. The simulations using parameter set #1 and set #2 are based on a uniform infiltration of 0.1 mm/yr, and the simulation results with parameter set #3 and set #4 use infiltration map #1 and map #2, respectively.

In the following analysis, only one of the four comparisons carried out for each borehole is presented in the figures, because the comparisons are all similar in matching the observation data.

8.6.1 Comparisons with UZ-1/14 Data

Boreholes UZ-1 and UZ-14 are adjacent to each other in Drill Hole Wash, north of the potential repository area (Figure 8.3.1), with surface elevations of about 1,349 m above sea level. A possible perched water zone was detected in or just below the base the Topopah Spring Tuff at a depth of 387 m. Comparisons were made between the simulated and observed saturation and capillary pressure (water potential) data for boreholes UZ-1/14, using the 4 different parameter sets of Section 8.5. Since similar comparison results were obtained using these 4 sets of parameters, only one of the comparisons is shown in Figure 8.6.1. In this figure, the vertical saturation profiles simulated are extracted from the 3-D simulation results, and the borehole data are from UZ-14. As shown on the figure and for all other results, the simulation results are generally in good agreement with the measured saturation profiles at the location of UZ-14, but comparisons with capillary pressure data are not as good as for saturation. The reason of this discrepancy between the simulated and observed capillary data may be due to the inaccuracy in the measurement of these water potential data ranging from sample handling to equipment limitations.

Figure 8.6.1

Comparisons of the simulated and observed saturations and water potentials of boreholes UZ-1/14 using parameter set #4 and infiltration map #2; (a) comparisons with saturation, (b) comparisons with capillary pressure. USGS data from L. Flint.

Figure 8.6.1 shows that the TCw unit is missing at this location. We have found that all four sets of parameters can match well with the saturation profiles from the ground surface until the bottom of the TSw unit in UZ-14. However, at the perched water location, as circled on the figure, the model results on Figure 8.6.1 fit better than models using the other sets of parameters. The comparisons in the altered CHnz unit also seem reasonable, considering the relatively coarse grids used in the 3-D model.

8.6.2 Comparisons with NRG-7a Data

Borehole NRG-7a is also located in Drill Hole Wash, and it is close to the ESF (Figure 8.3.1) at a surface elevation of 1,282 m. Perched water was also detected in this borehole, just below the contact of the bedded tuff with the partially welded pyroclastic flow at the base of the Topopah Spring Tuff. The comparisons between the simulated and observed saturations at the location are shown in Figure 8.6.2, as an example, for set #1 parameters. Since no water potential data are available from this borehole, only simulated capillary pressure data are plotted in the figure.

Figure 8.6.2

Comparisons of the simulated and observed saturations of borehole NRG-7a using parameter set #1 and infiltration of 0.1 mm/yr; (a) comparisons with saturation, (b) capillary pressure.

Figure 8.6.2 and the other results (Figures not given here) show that the simulated saturations are in a fair agreement with the observed values. The simulated saturation profiles are a little "wetter" than observed data. This may be due to the quality of the measured data; there are indications that the sample cores taken from the borehole were not handled properly, which decreases saturations (Personal Communication, USGS, L. Flint, 1996).

8.6.3 Comparisons with SD-7 Data

Borehole SD-7 is located near the southwest corner of the ESF, just west of the Ghost Dance fault (Figure 8.3.1). The offset in the geologic layering due to the fault is estimated to be on the order of tens of meters. A perched water body was found in the portion of the zeolitic Calico Hills tuff of the CHnz unit. An example of the comparison is shown in Figure 8.6.3 for borehole SD-7. It shows that the matches of the simulated and observed saturations and water potentials are good. For the upper three geological units, i.e., TCw, PTn, and TSw, the four sets of parameters and infiltration rates all results in good match with the observed data. However, the match with saturations in the CHnv units is not very good when using parameter set #1, or parameter set #3. Figures 8.6.3, using parameter set #4, gives a better fit with saturations in this unit, specially in the vitric layers above and below the perched water location, which is indicated by the circle in the figure.

Figure 8.6.3

Comparisons of the simulated and observed saturations and water potentials of borehole SD-7 using parameter set #4 and infiltration map #2; (a) comparisons with saturation, (b) comparisons with capillary pressure.

Different from all the other perched water boreholes discussed in this report, the perched-water body found in SD-7 is located within the Calico Hills zeolitic unit, in the middle of the CHn, rather than at the bottom of the welded tuff layer of the Topopah Spring unit. As shown in Figures 8.6.3, the perched-water location is reproduced well, and the resulting analysis indicates that use of parameter sets #1, #3 or #4 will better match the perched-water from the borehole. In these three comparisons, much higher saturation and lower capillary pressure values are obtained in the model results.

8.6.4 Comparisons with SD-9 Data

Borehole SD-9 is located adjacent to Drill Hole Wash (Figure 8.3.1) with a surface elevation of 1,302 m and has a total depth of 678 m. The perched water was found at a depth of 413 m, about 3 m above the lower nonlithophysal/vitrophyre contact in the Topopah Spring Tuff. The perched water zone was near the upper contact of the basal vitrophyre of the Topopah Spring Tuff in highly fractured, welded tuff underlain by less-fractured, non-welded tuff.

Figure 8.6.4 shows that the comparisons of the observed saturations and the modeled simulations. Also the results using the other three sets of parameters are similar to those in Figure 8.6.4. The figure indicates a good match for this borehole for all the geological units, except at the interface between the TSw and CHn units. At this interface, the observed saturations are as low as 40 - 50%, but the model gives values that are higher at 90% or more. The reason for

this disagreement may be the rock properties used for this layer. Since this zone is at the perched elevation, as shown in the figure, all the parameter sets were estimated to match the perched water of the borehole by the ITOUGH2 code (Chapter 3, Bandurraga et al.). Therefore, the model results are forced to produce higher saturations at this location. The other reason is the use of the coarse grid in the model, which leads to loss of resolution at the interfaces.

Figure 8.6.4
Comparisons of the simulated and observed saturations and water potentials of borehole SD-9 using parameter set #4 and infiltration map #2; (a) comparisons with saturation, (b) comparisons with capillary pressure.

It is interesting to note that there is a spike in the simulated saturation profiles, near the bottom of the model grid, or the water table. This is due to the presence of a thin layer of the Prow Pass vitric unit that is found there. In terms of matching the perched water location, Figure 8.6.4 using parameter set # 4 and map #2 infiltration rates gives the best fit for both saturation and capillary pressure profiles.

8.6.5 Comparisons with SD-12 Data

Borehole SD-12 is located near the center of the site-scale model (Figure 8.3.1), between the potential repository and the Exploratory Study Facilities (ESF). The borehole is at a surface elevation of 1,324 m and has a total depth of 660 m. The example simulation comparison results using are shown in Figure 8.6.5 for borehole SD-12. The figure gives comparisons only for saturations, since no water potential data are available for this borehole.

The match of the simulated salutations with the observed values is very reasonable for all the units, as shown in Figures 8.6.5, in particular, for the TSw

unit. In the PTn, the model predicted a lower saturation zone which is a little "thinner" than the observations. In the CHn, the two lower saturation spikes are reproduced well by the all the plots for the altered vitric zones, however, the model predictions are relatively "wetter" than the observed saturations there.

Figure 8.6.5

Comparisons of the simulated and observed saturations and water potentials of borehole SD-12 using parameter set #1 and infiltration of 0.1 mm/yr; (a) comparisons with saturation, (b) comparisons with capillary pressure.

8.6.6 Comparisons with UZ#16 Data

Borehole UZ#16 is located east of the potential repository, near the center of the ESF loop (Figure 8.3.1). UZ#16 is at a surface elevation of 1,219 m and has a total depth of 514 m. The simulation and comparison results using parameter set #4 are shown in Figure 8.6.6 for borehole UZ#16. The figure also gives comparisons only for saturations, since no measured water potential data are available for this borehole.

Figure 8.6.6

Comparisons of the simulated and observed saturations of borehole UZ#16 using parameter set #4 and infiltration map #2; (a) comparisons with saturation, (b) capillary pressure.

Figure 8.6.6 shows that the overall agreement of the simulated and measured saturation profiles at the location of UZ#16 is good, for all the units. Good agreement was observed for the other sets of parameters also. The match is very good for the lower saturation spike at the bottom of the model domain, which correspond to the unaltered layer of the Prow Pass Tuff in the CHn unit. The comparisons in the zeolitic units of the CHn show relatively large disagreement, because the model predicted values are a little "drier" than the observations. But the simulation results of Figure 8.6.6 using parameter set #4 and infiltration map #2 present a good fit in this zeolitic zone.

8.6.7 Comparisons with NRG-6 Data

Borehole NRG-6 is also located within the ESF loop (Figure 8.3.1), southeast of borehole NRG-7a and SD-9. NRG-6 has a surface elevation of 1,247 m and a total depth of 335 m. The example simulation and comparison results for borehole NRG-6 shown in Figure 8.6.7. There is no measured water potential data available for this borehole.

Figure 8.6.7

Comparisons of the simulated and observed saturations of borehole NRG-6 using parameter set #1 and infiltration of 01. mm/yr; (a) comparisons with saturation, (b) capillary pressure.

Figure 8.6.7 shows that the overall agreement of the simulated and measured saturation profiles at the location of NRG-6 is good, for all the units. However, the simulated saturations are a little "wetter" than the observations for this borehole. As discussed for NRG-7a borehole, the "wet" simulation results may be actually due to the quality of the sample measurement, because of mishandling the core samples (Private Comm., L. Flint, USGS, 1996).

8.7 Effects of Rock Property Variations on Moisture and Heat Flow

The effects of rock properties and their variations on moisture and heat flow and distributions within the mountain can be investigated using 2-D contour maps and 3-D plots. In this section, both 2-D and 3-D plots are used to analyze moisture flow fields and their spatial distributions, and to discuss lateral diversion issues.

8.7.1 Lateral Moisture Movement and Distribution in Selected 2-D Vertical Cross Sections

Figure 8.7.1 shows the location of four vertical cross sections, used to study moisture flow and distributions along these cross sections. The four vertical cross sections are selected to intersect boreholes UZ-14 and SD-7, from west to east, and south to north, respectively. All of the plots discussed in this Chapter are extracted from and based on 3-D simulation results.

Figure 8.7.1
Location and plan view of four vertical cross sections and associated boreholes.

8.7.1.1 Near Boreholes UZ-1/14

Figures 8.7.2 to 8.7.5 show the simulated flow velocity fields and liquid saturations along the vertical, west-east cross section W-E (UZ-1/14). The simulations use the four different sets of parameters and the corresponding infiltration rates. It is obvious from the figures that there exist significant differences in the lateral moisture movement predicted by the different sets of parameters and infiltration rates.

Figure 8.7.2

Velocity fields and liquid saturations along the West-East cross section crossing UZ-1/14, simulated using parameter set #1 and infiltration of 0.1 mm/yr.

Figure 8.7.3

Velocity fields and liquid saturations along the West-East cross section crossing UZ-1/14, simulated using parameter set #2 and infiltration of 0.1 mm/yr.

Figure 8.7.4

Velocity fields and liquid saturations along the West-East cross section crossing UZ-1/14, simulated using parameter set #3 and infiltration map #1.

Figure 8.7.5

Velocity fields and liquid saturations along the West-East cross section crossing UZ-1/14, simulated using parameter set #4 and infiltration map #2.

The velocity field, particle traveling paths and saturation contours, shown in Figure 8.7.2, are simulated using parameter set # 1 and a uniform infiltration rate of 0.1 mm/yr. Figure 8.7.2 shows significant lateral moisture flow in the west-east cross section both along the PTn and above the zeolitic units of the

CHnz, especially within the PTn. Figure 8.7.2 indicates that almost all the infiltration has been diverted laterally across three kilometers to the east in the PTn along the cross section, starting from the Solitario Canyon fault. At about one kilometer from the eastern model boundary, flow lines become vertical. This is because there is a relatively highly saturated zone along the lateral east-flow horizons, and the capillary force gradients there force the flow toward the west or downward. The turning points of flow directions near the eastern model boundary, as shown in Figure 8.7.2 or 8.7.4, also correspond to a sudden change in slopes of geological layers. We are currently investigating this.

Along the top of the zeolitic units in the CHn, as shown in Figure 8.7.2, water is diverted to the east for about one kilometer. On Figure 8.7.2, the higher saturations are noticed for these zeolitic layers of CHnz, which match the perched water location in boreholes UZ-1/14.

Figure 8.7.3 presents the simulations using parameter set #2 and 0.1 mm/yr infiltration, and shows a very different picture, with respect with the lateral diversion of moisture flow through the PTn. The water particles, released from the ground surface, go straight down across the PTn until reaching the zeolitic layers in the CHn. Along the top surface of the zeolitic units in the CHn, the figure indicates significant lateral flow, moisture traveling hundreds of meters toward the east. The simulation (Figure 8.7.3) that is relatively "dry" at the perched water location from this simulation.

Figure 8.7.4 also shows significant lateral movement in the PTn, and the results are simulated using parameter set #3 and infiltration map #1. Figure 8.7.4 indicates that similarly to Figure 8.7.2, almost all the recharge, from the Solitario Canyon fault to east, has been diverted, in the PTn, laterally traveling three kilometers to the east along the cross section to about one kilometer from the eastern model boundary. For the same reason as in Figure 8.7.2, downward flow occurs there.

Flow path lines, as shown in Figure 8.7.4, in the CHn unit indicate that there is little lateral flow in this unit, at about 200 meters near borehole UZ-1/14. The figure also shows an extensive water body with high saturation near the perched water location.

Figure 8.7.5 shows the simulation results using parameter set #4 and infiltration map #2. It indicates that there is very little lateral flow in both PTn and CHn units, and flow is mostly straight down to the water table. Figure 8.7.5 is based on the highest infiltration rates (map #2) used in this study, with an average of 4.4 mm/yr over the model domain. The results of the simulated moisture movement indicate that higher infiltration promotes vertical flow, relative to lateral movement. Figure 8.7.5 also shows a large high saturation body around the perched water location of borehole UZ-1/14.

The moisture flow and its distribution in the south-north direction, along cross section: S-N (UZ-1/14), are shown in Figures 8.7.6 to 8.7.9. The cross section location is shown in Figure 8.7.1. The simulations are using the four different sets of parameters and the corresponding infiltration rates, respectively. Compared with the results in the west-east cross section of Figures 8.7.2 to 8.7.5, the lateral flow in the south-north direction in the vicinity of UZ-1/14 is relatively small in the PTn, because of the smaller slopes of the layers in the south-north direction.

Figure 8.7.6 Velocity fields and liquid saturations along the South-North cross section crossing UZ-1/14, simulated using parameter set #1 and infiltration of 0.1 mm/yr.

Figure 8.7.7 Velocity fields and liquid saturations along the South-North cross section crossing UZ-1/14, simulated using parameter set #2 and infiltration of 0.1 mm/yr.

Figure 8.7.8

Velocity fields and liquid saturations along the South-North cross section crossing UZ-1/14, simulated using parameter set #3 and infiltration map #1.

Figure 8.7.9

Velocity fields and liquid saturations along the South-North cross section crossing UZ-1/14, simulated using parameter set #4 and infiltration map #2.

Figure 8.7.6 shows about 100-300 meters lateral flow in the PTn unit, along the south-north cross section when using parameter set #1 and 0.1 mm/yr infiltration. However, substantial lateral movement can be seen in the CHn unit from south to north up to 700 meters. Figure 8.7.7 uses also 0.1 mm/yr infiltration, with parameter set #2. The picture is similar to that in the west-east direc-

tion (Figure 8.7.3). i.e., the only lateral flow occurs within the CHn, and flow is around the zeolitic unit. There is significant south-north flow, as shown in Figure 8.7.7, over a distance of more than 500 meters in the southern part of the cross section, under the repository horizon.

Using parameter set # 3 and infiltration map #1 in the model, Figure 8.7.8 shows moderate lateral moisture flow in the PTn for about 100 - 300 meters. The lateral movement and direction are similar to those shown in Figure 8.7.6. The lateral diversion within the CHn is also moderate, up to 300 meters to the north in the southern part of the cross section.

Figure 8.7.9 depicts the simulation results using parameter set #4 and infiltration map #2. The figure indicates that there is hardly any lateral flow along the south-north direction. It agrees with what is shown in Figure 8.7.5 under the same model condition.

8.7.1.2 Near Borehole SD-7

The simulated flow velocity fields and saturations along the west-east cross section: W-E (SD-7) are shown in Figures 8.7.10 to 8.7.13. The simulations use the same four sets of parameters. The lateral diversion in the vicinity of SD-7 is much smaller in the PTn than in the west-east cross section near UZ-1/14. This may be due to the PTn unit, which is much thinner near SD-7 than that near UZ-1/14. However, Figures 8.7.10 - 8.7.13 show that significant lateral diversions occur only in the CHn.

Figure 8.7.10
Velocity fields and liquid saturations along the West-East cross section crossing SD-7, simulated using parameter set #1 and infiltration of 0.1 mm/yr.

Figure 8.7.11

Velocity fields and liquid saturations along the West-East cross section crossing SD-7, simulated using parameter set #2 and infiltration of 0.1 mm/yr.

Figure 8.7.12

Velocity fields and liquid saturations along the West-East cross section crossing SD-7, simulated using parameter set #3 and infiltration map #1.

Figure 8.7.13

Velocity fields and liquid saturations along the West-East cross section crossing SD-7, simulated using parameter set #4 and infiltration map #2.

Figures 8.7.10, 8.7.11, and 8.7.12 show the results of simulations using parameter sets #1, #2 and #3, respectively. They all indicate that there is large lateral flow in the CHn between the Solitario Canyon and Ghost Dance faults, with lateral diversion of 100 to 1,000. Figures 8.7.10 and 8.7.12 also show higher saturations along the base of TCw, indicating a capillary barrier along the interface. Also, as shown in these figures, east of the Ghost Dance fault, the diverted moisture tends to flow to the Bow Ridge fault along the cross section.

Similar to the flow shown the UZ-1/14 W-E cross-section, the model using parameter set #4 and infiltration map #2 gives results showing little lateral diversion in all the units (Figure 8.7.13).

Figures 8.7.14 to 8.7.16 show the results along the south-north direction in the vicinity of SD-7. Figure 8.7.14 indicates that lateral diversions of moisture occur only in the top portion, a vitric layer, of the CHn unit, between SD-7 and SD-12. The total travel distance is about 500 meters to the north along this vitric layer.

Figure 8.7.14

Velocity fields and liquid saturations along the South-North cross section crossing SD-7, simulated using parameter set #1 and infiltration of 0.1 mm/yr.

Figure 8.7.15

Velocity fields and liquid saturations along the South-North cross section crossing SD-7, simulated using parameter set #2 and infiltration of 0.1 mm/yr.

Figure 8.7.16

Velocity fields and liquid saturations along the South-North cross section crossing SD-7, simulated using parameter set #3 and infiltration map #1.

Figure 8.7.17

Velocity fields and liquid saturations along the South-North cross section crossing SD-7, simulated using parameter set #4 and infiltration map #2.

Figure 8.7.15 shows a different lateral diversion in which flow is towards the south, along the vitric layer of the top of the CH pattern. The simulation results are based on parameter set #2 and 0.1 mm/yr infiltration. All the other results in Figures 8.7.14, 8.7.16, and 8.7.17 indicate that the water is diverted to the north along the same top vitric unit of the same cross section. It is very

interesting, as shown in Figure 8.7.15, to note that water is moving to the south in the upper vitric layer and then flows back to the north, once it is past the zeolitic, or crosses a thin zeolitic layer near SD-7. Further analysis shows that the significant lateral flow along the vitric layers is due to large capillary pressure gradients, which overcome gravity forces along the dipping layer to the north. It can be seen from Figure 8.7.15 that it gets "drier" in the south end of the cross section than in the north in the top vitric unit, and this indicates that the flow direction is determined by capillary forces.

Figure 8.7.16 shows a small lateral moisture movement within the CHn, with a distance of about 100 - 200 meters. Again, Figure 8.7.17, which uses parameter set #4 and infiltration map #2, results in little lateral diversions in any units of the formation.

In summary, this study indicates that there are significant effects of rock properties and infiltration rates on lateral moisture flow in the unsaturated zone of Yucca Mountain. The PTn unit may divert water thousands of meters laterally to the east at certain locations of the mountain, and the extent of the simulated lateral movement within the PTn depends mainly on the rock properties, infiltration rates, and conceptual geological model. The lateral diversion of water flow in the unsaturated zone at Yucca Mountain is a complex phenomenon, as indicated by the 3-D modeling results. However, the key factors that have been observed to affect water lateral movement within the mountain the most are "capillary barrier" effects (Oldenburg and Pruess, 1993) and infiltration rates applied on the ground surface. This is especially true for the PTn unit, as shown in the figures discussed in this section. Permeability in the PTn unit is several orders of magnitude higher than that for the unit (TCw) above or the unit (TSw) below, but the capillary forces or the air entry pressures are not much different (See Tables 8.5.1 - 8.5.4 for the 4 sets of parameters). Therefore, a very "dry" zone may be created along the PTn, compared with those in the layers above and below from all the simulations. Thus a strong capillary barrier effect is expected across the PTn. The capillary effects change with the contrasts in moisture contents of the PTn and the adjacent units, which are directly related to the infiltration rates on the ground surface. Once a layer with strong capillary forces overlies a low capillarity layer and the vertical capillary gradients for upward water flow are large enough to overcome the gravity forces, the water flow only occurs in the lateral direction. This explains why there is hardly any lateral movement in the PTn when an infiltration rate is larger than 1 mm/yr from the modeling results.

In addition to large lateral flow in the PTn unit observed in some of the simulations, substantial lateral diversions also occur around the zeolitic units in the CHn formation. The strong moisture lateral movement in the CHnz unit, predicted in the 3-D simulation, is consistent with the thermal analysis results in Chapter 9 (Bodvarsson et al.). The lateral movement within the CHn unit tends

to divert water east to the Bow Ridge fault, along the dipping slopes of the zeolitic units.

8.7.2 3-D Lateral Moisture Distributions and Movement

The moisture movement and distribution within the mountain can be seen more intuitively using 3-D plots. In this section, we present some of the 3-D simulation results using 3-D perspective pictures for saturations and velocity components in different directions.

The 3-D plots of saturations, simulated using parameters set #1 and #4, 0.1 mm/yr and map #2 infiltration rates, respectively, are shown Figures 8.7.18 and 8.7.19. It should be mentioned that the figures, such as Figures 8.7.19 and 8.7.20, which show the simulation results at the repository horizon, are based on the information of the model layer that represents the repository. The model layer for the repository is relatively flat only in the area of the repository, and its elevation and thickness vary outside the repository.

Figures 8.7.18 and 8.7.19 indicate a very non-uniform, but similar distribution of liquid saturations at the repository horizon. Along the four faults, Solitario Canyon, Iron Ridge, Ghost Dance and Abandoned Wash, and Dune Wash faults, very "dry" unsaturated zones are shown on the figures. In the case of lower infiltration, 0.1 mm/yr, Figure 8.7.18 shows an average saturation ranging from 0.4 to 0.6 at the potential repository between the Solitario Canyon fault and boreholes SD-7, SD-12, and SD-9. For a higher infiltration rate of map #2, Figure 8.7.19 gives a slightly higher saturations, ranging from 0.5 to 0.7 at the repository level.

Water Saturation at Repository Horizon

Figure 8.7.18

Saturations at the repository horizon and below, simulated using parameter set #1 and infiltration of 0.1 mm/yr.

Water Saturation at Repository Horizon

Figure 8.7.19

Saturations at the repository horizon and below, simulated using parameter set #4 and infiltration map #2.

Figure 8.7.20 shows a 3-D profile of saturations, with a volume cut along the west-east section, crossing UZ-1/14, then to the south, crossing SD-9, SD-12, and SD-7. The figure shows clearly certain high saturation zones on both sides of the Solitario canyon fault, and along the south-north cut section. The latter corresponds to the lower part of the TSw, west of the Ghost Dance fault, and the zeolitic units in the CHn.

Figure 8.7.20

Saturations at the repository horizon and below, simulated using parameter set #4 and infiltration map #2.

The lateral diversions of moisture flow by the PTn can be seen using 3-D plots of velocity components in different directions. We also use the simulation results from parameter sets #1 and #4, since these two sets of parameters produce very different lateral movement along the PTn, as discussed above. The three velocity components of flow fields simulated using parameter set #1 and #4 are shown in Figures 8.7.21 to 8.7.26, respectively. In these figures, units of scales in legends denote mass fluxes in terms of mm/yr for comparison with infiltration rates imposed on the top surface boundary

Figure 8.7.21 shows the west-east lateral mass fluxes at the middle of the PTn. On this figure and others showing west-east flow components, positive "values" or red colors indicate flow to the east directions, and the negative "values" or blue colors show west-bound flow. Figure 8.7.21 shows very large lateral flow from west to east within the PTn in the northern part of the model domain on both sides of the Solitario Canyon fault, especially near the bore-

holes UZ-1/14 and SD-9, on the order of 2 mm/yr. This result is consistent with the 2-D cross section analysis, as shown in Figure 8.7.2. Figure 8.7.21 indicates clearly that the lateral moisture flow within the PTn is dominantly from west to east, because slopes or dips of geological layers mostly are along the west-east direction.

West-East Mass Flux at Middle of PTn

Figure 8.7.21

Velocity components in the west-east direction at the middle of the PTn, and below, simulated using parameter set #1 and infiltration of 0.1 mm/yr.

Figures 8.7.22 and 8.7.23 shows south-north and vertical components of moisture flow within the PTn, respectively. On Figure 8.7.22 or other south-north flow component plots, positive values or red color indicate south-bound flow, and negative values or blue colors show flow to north. On vertical flow maps, such as Figure 8.7.23, negative values denote downward flow. The simulation results in Figure 8.7.22 shows that there is very small lateral movement in the south-north direction in most of the PTn unit, except in the northern part of the domain, where significant north-bound flow occurs west of the Solitario Canyon fault and at the north-east corner of the model.

The vertical flow, as shown in Figure 8.7.23, indicates very non-uniform percolation fluxes crossing the PTn, even though a uniform surface infiltration rate, 0.1 mm/yr is used in this case. An averaged flux value of 0.1 to 0.2 above the repository can be seen from Figure 8.7.23, but in the northern part of the

domain, west of the Solitario Canyon fault and around the north-east corner of the model, significantly higher vertical fluxes, at about 4 mm/yr, are obtained in the simulation. This is due to the huge lateral diversion of flow toward these areas, as shown in Figures 8.7.21 and 8.7.22.

South-North Mass Flux at Middle of PTn

Figure 8.7.22

Velocity components in the south-north direction at the middle of the PTn, and below, simulated using parameter set #1 and infiltration of 0.1 mm/yr.

West-East Mass Flux at Middle of PTn

Figure 8.7.24 Velocity components in the west-east direction at the middle of the PTn, and below, simulated using parameter set #4 and infiltration map #2.

South-North Mass Flux at Middle of PTn

Figure 8.7.25 Velocity components in the south-north direction at the middle of the PTn, and below, simulated using parameter set #4 and infiltration map #2.

Figure 8.7.26
Velocity components in the vertical direction at the middle of the PTn, and below, simulated using parameter set #4 and infiltration map #2.

In summary, the 3-D plots of the two simulations indicate that very different percolation fluxes and lateral movement in the PTn are obtained when using different infiltration maps and rock properties. The higher infiltration rates tends to promote more vertical flow than lateral movement in the PTn unit. The percolation fluxes across the PTn unit are mainly from the lateral diversion in the lower infiltration case studied. The flux pattern follows the surface infiltration pattern when using infiltration map #2.

8.7.3 Ambient Geothermal Conditions and Heat Flow at Repository Horizon

The temperature distributions within the mountain, simulated by the four sets of rock properties and infiltration rates, are similar, and therefore, we present only one 3-D temperature plot (Figure 8.7.27). The volume cut at the south-west part of the model, as shown in Figure 8.7.27, indicates that temperature is at about 25 degree-C at the repository level.

Figure 8.7.27

3-D temperature distributions in the unsaturated zone of Yucca Mountain, simulated using parameter set #4 and infiltration map #2.

A vertical heat flow map, showing heat flux in W/m^2 at the repository horizon is shown in Figure 8.7.28. All the simulations conducted produce a heat flow pattern at the repository horizon similar to that shown in Figure 8.7.28. The averaged heat flow value is about 30 to 40 mW/m^2 , which is consistent with the estimation by Sass et al. (1988). The figures show that the highest heat flow occurs at the south-west corner of the model, where the ground surface elevation is the lowest, and the water table temperatures are the highest (Section 8.3.3). Few blue spots on the heat flow maps correspond to the low upward heat flow rates, which correlate with the higher percolation fluxes in these areas. The convection heat transfer by percolation is always downwards, therefore, as expected, the total upwards heat flow is the combined result of heat conduction and convection by liquid and vapor, and it becomes lower where the percolation flux is high. Detailed analysis of percolation fluxes from temperature data are given in Chapter 9 (Bodvarsson et al.).

Figure 8.7.28

Vertical heat flow map at repository horizon of the unsaturated zone of Yucca Mountain, simulated using parameter set #4 and infiltration map #2.

8.8 Effects of Fault Properties

Three sets of fault properties, as summarized in Section 8.5.6, have been used in this Chapter to investigate effects of these fault properties on moisture flow in the unsaturated zone of Yucca Mountain. The fault properties were based on the previous modeling studies (Wittwer et al., 1995; and Ahlers et al., 1995 a and b) at LBNL, and the recent pneumatic analysis results (Ahlers et al., 1996). The major faults incorporated into the site-scale model are shown in Figure 8.3.1, which include the Solitario Canyon, Iron Ridge, Ghost Dance and Abandoned Wash, and Dune Wash faults. The Bow Ridge fault is treated as a boundary condition along the eastern boundary of the model domain.

The faults are represented in the model as vertical zones with consideration of stratigraphic offsets, connections to adjacent gridlayers, and variable thickness. In addition, fracture and matrix flow within fault zones are treated using the ECM approximation, instead of a single continuum porous medium, as in the previous study (Wittwer et al., 1993 and 1995).

The purpose of this section is to present sensitivity analyses of effects of fault properties on 3-D moisture flow within Yucca Mountain. The representative values of fault rock properties used in the sensitivity study are listed in Table 8.5.6, 8.5.7 and 8.5.8 for property sets of fault #1, fault #2, and fault #3, respectively, in Section 8.5.6.

8.8.1 W-E Cross Section at SD-7

The fault #1 properties, listed in Table 8.5.6, use a set of uniform fault rock parameters for all the incorporated faults, and this set of fault properties has been used in most of the simulations reported this Chapter. The effects of fault properties on moisture flow can be seen clearly from the west-east vertical cross sections, as shown in Figures 8.8.1 to 8.8.4. The moisture flow and roles played by the three major faults, the Solitario Canyon, Ghost Dance and Dune Wash faults, along the west-east (SD-7) cross section (Figure 8.7.1), are displayed in these figures. The simulations for these figures are based on fault #1 properties, and parameter sets #1 to #4 with the corresponding infiltration rates, respectively.

Figure 8.8.1
Moisture movement and distributions along the West-East cross section crossing SD-7, Solitario Canyon, Ghost Dance and Dune Wash faults, simulated using fault #1 properties, parameter set #1 and infiltration of 0.1 mm/yr.

Figure 8.8.2

Moisture movement and distributions along the West-East cross section crossing SD-7, Solitario Canyon, Ghost Dance and Dune Wash faults, simulated using fault #1 properties, parameter set #2 and infiltration of 0.1 mm/yr.

Figure 8.8.3

Moisture movement and distributions along the West-East cross section crossing SD-7, Solitario Canyon, Ghost Dance and Dune Wash faults, simulated using fault #1 properties, parameter set #3 and infiltration map #1.

Figure 8.8.4

Moisture movement and distributions along the West-East cross section crossing SD-7, Solitario Canyon, Ghost Dance and Dune Wash faults, simulated using fault #1 properties, parameter set #4 and infiltration map #2.

Figures 8.8.1 to 8.8.4 show that the three south-north faults (the Solitario Canyon, Ghost Dance, and Dune Wash) all act as a capillary barrier to the lateral moisture flow along this cross section. The faults stay relatively "dry" with saturations of 10 - 20% when using this set of fault properties. The figures also indicate that the vertical flow paths near the faults are mainly parallel to the faults. However the moisture flow may cross or leave the faults laterally at several locations, as indicated in the four figures. Flow leaves or crosses the Solitario Canyon and Dune Wash faults at the interfaces between TCw and PTn, and moves towards the east. In these locations large offsets exist, and the PTn units on both sides of the faults are completely separated, while the TCw and the TSw formations are connected through fault zones.

Along part of the Ghost Dance fault, the vertical flow is also diverted laterally to the east near the interface of the TSw and CHn, due to high saturation zones on both sides of the fault, as shown in Figures 8.8.1, 8.8.3 and 8.8.4.

Figure 8.8.5 shows the simulation results using fault #2 properties and parameter set #1 with a uniform infiltration of 0.1 mm/yr. As discussed in Section 8.5, the only difference between fault #2 and fault #1 properties is in absolute fracture permeability. Fault #2 properties use four different fracture permeabilities for the four vertical geological units of faults, respectively, instead of a uniform fracture permeability as in fault #1 properties. The fracture permeability values are derived from the pneumatic analysis (Ahlers et al.,

1996). A comparison of Figures 8.8.5 and 8.8.1 indicates that very similar results are obtained using fault #1 and fault #2 properties. The only noticeable difference in predicting moisture flow using these two sets of fault properties is in the Dune Wash fault, at the middle of CHn, where Figure 8.8.5 shows a flow path line crossing the fault. This is because a much lower fracture permeability value of 10 md is used for the faults within the CHn unit in fault #2. Overall, Figure 8.8.5 and 8.8.1 show that differences in absolute fracture permeability of fault zones have little effects on moisture flow near faults.

Figure 8.8.5

Moisture movement and distributions along the West-East cross section crossing SD-7, Solitario Canyon, Ghost Dance and Dune Wash faults, simulated using fault #2 properties, parameter set #1 and 0.1 mm/yr infiltration.

Figure 8.8.6 shows the flow along the same west-east cross section, and the simulation results are based on all the rock properties (parameter set #4), as used for Figure 8.8.4, except that fault #3 replaces fault #1 properties (Figure 8.8.4). Fault #3 properties are different from the set of fault #1 not only in fracture permeability, but also in moisture retention functions for fault zones. As shown in Table 8.5.8, much stronger capillary suctions are provided by the fault #3 properties, which were selected from van Genuchten parameters estimated in parameter set #4 for corresponding units.

A comparison of Figures 8.8.6 and 8.8.4 indicates that there is a significant difference in saturations along the faults. Figure 8.8.6 gives much "wetter" conditions at or near faults, with saturation values between 40 to 80%. This is due to the higher capillary suctions within the matrix material of faults. As a result, faults shown in Figure 8.8.6 do not act as capillary barriers anymore. Instead, the faults with fault #3 properties and higher infiltration map #2 behave as a conduit for nearby moisture flow because of relatively higher permeability and strong capillary pressure forces along the faults.

Figure 8.8.6

Moisture movement and distributions along the West-East cross section crossing SD-7, Solitario Canyon, Ghost Dance and Dune Wash faults, simulated using fault #3 properties, parameter set #4 and infiltration map #2.

8.8.2

W-E Cross Section at UZ-1/
14

For the west-east cross section of UZ-1/14 (Figure 8.7.1), Figures 8.8.7 and 8.8.8 show very similar moisture flow fields and liquid saturation contours when using fault #1 and #2 properties, with the same infiltration and rock parameter set. The Solitario Canyon faults on the two figures are both "dry", acting as a capillary barrier to lateral moisture flow. However, a flow path leaves the fault, and is diverted to the east at near the interface of the TSw and CHn units (Figure 8.8.8), using the fault #2 properties, for the same reasons discussed previously.

Figure 8.8.7

Moisture movement and distributions along the West-East cross section crossing UZ-1/14 and Solitario Canyon fault, simulated using fault #1 properties, parameter set #1 and infiltration of 0.1 mm/yr.

Figure 8.8.8

Moisture movement and distributions along the West-East cross section crossing UZ-1/14 and Solitario Canyon fault, simulated using fault #2 properties, parameter set #1 and infiltration of 0.1 mm/yr.

Figures 8.8.9. and 8.8.10 show a comparison of the simulation results using the fault #1 and #3 properties, and infiltration map #2 and rock parameter set #4, respectively. Similar to the W-E cross section of SD-7, Faults #1 and #3 with

parameter set # 4 and high infiltration rates of map #2 result in very different predictions on the role of faults. Figure 8.8.9 shows that the Solitario Canyon fault is very "dry", and acts as a capillary barrier, while Figure 8.8.10 indicates a very "wet" fault that carries water down to the water table.

Figure 8.8.9

Moisture movement and distributions along the West-East cross section crossing UZ-1/14 and Solitario Canyon fault, simulated using fault #1 properties, parameter set #4 and infiltration map #2

Figure 8.8.10

Moisture movement and distributions along the West-East cross section crossing UZ-1/14 and Solitario Canyon fault, simulated using fault #3 properties, parameter set #4 and infiltration map #2.

8.8.3 Groundwater Travel Times

The water ages estimated from perched water samples from UZ-14 and SD-7, based on ^{14}C data (Rousseau et al., 1996; Luckey, 1995), could give us an independent check of the water traveling times simulated in our model calibration and sensitivity studies. It was estimated that the ages of perched water from boreholes UZ-14 varied between 5,150 and 11,000 years old (Rousseau et al., 1996). The perched water of SD-7 may be 3,000 to 7,000 years old (Yang et al., 1996). The data on the SD-7 perched water age are in the process of being qualified by the USGS.

Using the 3-D modeling results of this Chapter and a particle tracking scheme, we can also estimate the ages of the water at the perched water locations. Near UZ-1/14, total time for water to travel from the surface to the perched level is about 5,000 - 10,000 years, for the simulations based on the different parameter sets, but high infiltration scenarios, and fault #1 or #3 properties. These estimated water ages is consistent with the 5,150 to 11,000 years by the geochemistry data.

Using the higher infiltration rates, the ages of the perched water at SD-7 can be estimated at about 5,000 to 12,000 years, which is somewhat consistent with the isotopic ages of 3,000 to 7,000 years. Perched water issues are discussed in Chapter 7 (Wu et al., 1996) of this report.

8.9 3-D Dual-Permeability Model

As part of model sensitivity analyses described in this report, a three-dimensional dual-permeability model has been developed and is presented in this section. The dual-permeability model is an alternate conceptual model that can be used to study fracture/matrix flow phenomena at Yucca Mountain. It is a built-in option in the TOUGH2 code and has been qualified for use in the Yucca Mountain Project. The details of the dual-permeability approach can be found in Pruess and Narasimhan (1985) and Pruess (1983, 1991).

8.9.1 Dual-Permeability Model Grid and Parameters

The dual-permeability model discussed in this section extends over the entire 3-D model domain and grid (Figure 8.3.1). The dual-permeability grid was derived using the 3-D grid shown in Figure 8.3.1 as a primary grid. All the connection information, such as fracture-fracture, fracture-matrix, and matrix-matrix connecting areas and distances, were calculated using the MINC approach (Pruess, 1983). We did not reduce the connection areas between fracture and matrix elements as done by Ho et al. (1995). The fracture system in the unsaturated zone of the mountain is subdivided into four zones, which corresponds to the hydrogeologic units, TCw, PTn, TSw and CHn, respectively. The properties of the fractures for the four units are taken from TSPA-93 (Wilson et al., 1994), as listed in Table 8.9.1. Since few fractures through-going exist in the PTn unit, the effects of fractures on moisture flow in the PTn are ignored in this

study, and the PTn formation is treated as a single porous medium. Also, the fracture/matrix flow in the fault zones, shown in Figure 8.3.1, is treated using the ECM approach. This may be a reasonable assumption, because matrix block sizes are smaller within fault zones than in fractured rocks outside, and the ECM equilibrium condition is better satisfied in the fault zones.

Table 8.9.1 The fracture porosity, aperture and spacing data used for the dual-permeability simulations (Wilson et al., 1994).			
Unit	Porosity	Aperture (m)	Spacing (m)
TCw	1.38e-3	0.181e-3	.618
PTn	4.12e-3	0.206e-3	2.22
TSw	2.75e-3	0.180e-3	.740
CHn	9.98e-4	0.179e-3	1.618

In the dual-permeability simulations, parameter set # 4, for matrix and fractures, and infiltration map #2 are used, as listed in Table 8.5.4. The same boundary conditions and specifications, as described in Section 8.3, are used here. However, the water infiltration on the ground surface was only added into the fracture elements at the top boundary, and isothermal conditions were assumed to exist under two-phase flow conditions.

8.9.2 Comparisons with the ECM Results

A systematic study is presented in this section for comparing the results using the dual-permeability and ECM approaches on the large scale, 3-D, site-scale model. The simulation results are compared using liquid saturations and capillary pressure of fracture and matrix, obtained using both methods. Comparisons are also made with the observed matrix saturation data from several boreholes. The measured saturation data are from 7 boreholes UZ-14, UZ-16, NRG-6, NRG-7a, SD-7, SD-9, and SD-12, collected by the USGS (OCRWM, DOE, 1995).

We present the results of simulations and comparisons only for borehole SD-7, because for all the other boreholes, almost the same results are obtained. Figures 8.9.1 and 8.9.2 show the comparisons of vertical saturation and capillary pressure profiles in the matrix and fractures for borehole SD-7, including observations (if available) and simulated values using the dual-permeability and ECM approaches. It should be mentioned that the saturations in the PTn unit, shown in the figures, are for matrix only, since this unit is treated as a single continuum porous medium. The same saturations are also used in plots of fracture saturations for producing continuous curves vertically.

Figure 8.9.1 shows that almost identical results of both matrix saturations and capillary pressures are obtained from the two modeling approaches. The only differences between the two solutions may be noticed in the TCw unit, or

along the interfaces between PTn and TCw or TSw. The reasons for this minor difference are due to the conceptual model used, rather than the modeling approaches. First, in the dual-permeability simulation the water infiltration is injected into fractures only on the top boundary, while the ECM model puts the infiltration into both fracture and matrix systems. Secondly, in the dual-permeability model the top and the bottom gridlayers in the PTn unit are connected vertically only to the fracture elements in the TCw or the TSw, while the ECM model connects to both fractures and matrix. Therefore, there are discontinuities in matrix vertical connections across these interfaces. As can be seen from these figures, in the dual-permeability model water cannot flow into the PTn directly from matrix at the bottom of the TCw, and it must go through the fractures. As a result, matrix saturations simulated from the dual-permeability model are higher, or capillary pressures are lower at this interface than those in the ECM simulations.

Figure 8.9.1

Comparisons of the observed and simulated saturations and capillary pressures using dual-permeability and ECM approaches at borehole SD-7 with parameter set #4 and infiltration map #2; (a) matrix saturation, (b) matrix capillary pressure.

A comparison of simulated fracture saturations at borehole SD-7 is shown in Figure 8.9.2, and the results are from the dual-permeability and the ECM approaches, respectively. Again the two solutions for fracture saturations are in good agreement under the three-dimensional flow condition. Also comparisons of fracture saturations obtained from the two modeling approaches have been made for the other boreholes, and they all match well, as shown in Figure 8.9.2.

Figure 8.9.2
Comparisons of the observed and simulated fracture saturations using dual-permeability and ECM approaches at borehole SD-7 with parameter set #4 and infiltration map #2

8.9.3 Effects of Climate Changes Using High-Pulse Infiltration

In this section, a high-pulse infiltration scenario (climate change) is proposed using a much larger infiltration rate, i.e., three times higher than the averaged value used for infiltration map #2, or 13.2 mm/yr over the model domain. The use of such a high infiltration rate is reasonable according to Sheryl Morris of DOE (Personal Comm., 1996). The high-pulse infiltration rate is assumed for possible higher infiltration condition in the future due to climate changes. The initial condition for this high-pulse infiltration simulation is the steady-state condition generated by the previous dual-k run using the map #2 infiltration and parameter set #4. The infiltration rate is increased by a factor of three when the high-pulse simulation started.

The effects of high-pulse infiltration and transient simulations are analyzed using 2-D plots of moisture content and velocity distributions along the west-east vertical cross section crossing UZ-14 (Figure 8.7.1). The simulation results are shown in Figures 8.9.3 to 8.9.10 for simulation times of 100, 1,000, 30,000, and 100,000 years, respectively. The same scaling factors for the velocity vectors are used for matrix and fracture in all the figures.

Figures 8.9.3 and 8.9.4 show liquid saturations and velocity fields after 100 years for the matrix and fractures. As can be seen in these two figures, the high infiltration front has only moved down to the middle of the PTn unit. But along the Solitario Canyon fault, the water front has passed the PTn and entered the TSw.

Figure 8.9.3
Matrix liquid saturations and velocity fields after 100 years along the West-East cross section crossing UZ-1/14, simulated using a dual-permeability approach and high-pulse infiltration rate.

Figure 8.9.4
Fracture liquid saturations and velocity fields in 100 years along the West-East cross section crossing UZ-1/14, simulated using a dual-permeability approach and high-pulse infiltration rate.

Figures 8.9.5 and 8.9.6 show a much deeper penetration of the water front in both the fracture and the matrix systems, after 1,000 years. Figure 8.9.6 indicates (when compared with Figure 8.9.4 at 100 years) that the front already reaches the water table in the west half of the cross section through fractures in 1,000 years. The water flowing through the matrix also enters the CHn unit in 1,000 years, and reaches the water near the eastern boundary. Both of the figures show that the Solitario Canyon fault acts as a major flow pathway for rapid downward water movement. A comparison of Figures 8.9.5 and 8.9.3 show that the matrix in most of the cross section are much "wetter" at 1,000 years than at 100 years, as should be expected under the assumed infiltration condition.

Figure 8.9.5

Matrix liquid saturations and velocity fields in 1,000 years along the West-East cross section crossing UZ-1/14, simulated using a dual-permeability approach and high-pulse infiltration rate.

Figure 8.9.6

Fracture liquid saturations and velocity fields in 1,000 years along the West-East cross section crossing UZ-1/14, simulated using a dual-permeability approach and high-pulse infiltration rate.

After 30,000 years, higher flow velocities can be seen everywhere in both fractures and matrix, as shown in Figures 8.9.7 and 8.9.8, and both systems are somewhat "wetter" than after 1,000 years.

Figure 8.9.7

Matrix liquid saturations and velocity fields in 30,000 years along the West-East cross section crossing UZ-1/14, simulated using a dual-permeability approach and high-pulse infiltration rate.

Figure 8.9.8

Fracture liquid saturations and velocity fields at 30,000 years along the West-East cross section crossing UZ-1/14, simulated using a dual-permeability approach and high-pulse infiltration rate.

After 100,000 years, Figures 8.9.9 and 8.9.10 show that there is little difference, for both saturation and velocity distributions, in the cross section, from those observed after 30,000 years. Therefore, the system reaches a steady-state after approximately 30,000 years under the high-pulse infiltration conditions.

Figure 8.9.9

Matrix the saturations and velocity fields in 100,000 years along the West-East cross section crossing UZ-1/14, simulated using a dual-permeability approach and high-pulse infiltration rate.

Figure 8.9.10

Fracture liquid saturations and velocity fields in 100,000 years along the West-East cross section crossing UZ-1/14, simulated using a dual-permeability approach and high-pulse infiltration rate.

8.10 Simulations of Percolation Fluxes

The percolation fluxes at the repository horizon and the water table recharge maps are simulated using the 4 sets of parameters and the ECM and dual-permeability approaches. The results are presented and analyzed in this section. Among all the important factors which affect the repository performance, the percolation fluxes through the unsaturated zone of the mountain are the most critical for PA calculations, because spatial and temporal variations in percolation fluxes affect:

- (a) water flow into drifts;
- (b) corrosion environment in the canisters;
- (c) waste mobilization; and
- (d) waste migration to the saturated zone.

8.10.1 Percolation Fluxes at Repository Horizon

As part of the output of the sensitivity studies, the percolation fluxes at repository horizons and recharge maps at the water table were calculated, as shown in Figures 8.10.1 - 8.10.6. In these figures, the unit of mass fluxes is converted to mm/yr, as used for infiltration, and the "negative" values denote

downwards flow. All the percolation maps at the repository horizon (Figures 8.10.1 to 8.10.6) show very non-uniform flux distributions.

Figure 8.10.1 shows that the percolation fluxes near the repository area is about 0.05 to 0.1 mm/yr, which is close to the infiltration rate, 0.1 mm/yr used in this simulation. The dark blue spots on the figure indicate higher percolation fluxes, or preferential flow pathways at the repository horizon. These fast flow pathways can be easily identified on the figure.

Vertical Mass Flux at Repository Horizon

Figure 8.10.1

Percolation fluxes at the repository horizon, simulated using the ECM model, parameter set #1 and uniform infiltration rate of 0.1 mm/yr.

Vertical Mass Flux at Repository Horizon

Figure 8.10.2 Percolation fluxes at the repository horizon, simulated using the ECM model, parameter set #2 and uniform infiltration rate of 0.1 mm/yr.

Vertical Mass Flux at Repository Horizon

Figure 8.10.3 Percolation fluxes at the repository horizon, simulated using the ECM model, parameter set #3 and infiltration map #1.

Vertical Mass Flux at Repository Horizon

Figure 8.10.4 Percolation fluxes at the repository horizon, simulated using the ECM model, parameter set #4 and infiltration map #2.

Vertical Fracture Mass Flux at Repository Horizon

Figure 8.10.5 Fracture percolation fluxes at the repository horizon, simulated using the dual-permeability model, parameter set #4 and infiltration map #2.

Vertical Matrix Mass Flux at Water Table

Figure 8.10.6

Matrix percolation fluxes at the repository horizon, simulated using the dual-permeability model, parameter set #4 and infiltration map #2.

The percolation fluxes in Figure 8.10.2 shows a more uniform distribution than in Figure 8.10.1, even though in both cases the uniform infiltration rate is 0.1 mm/yr. A few light blue spots on Figure 8.10.2 identifies the fast flow paths through the repository horizon, but velocities are less than in the case shown in Figure 8.10.1.

Figure 8.10.3 shows very non-uniform percolation fluxes. The average value of vertical mass fluxes near the repository area is about 0.1 to 0.15 mm/yr, which is lower than the average infiltration from map #1. Also, a few dark blue areas indicate the fast flow pathways.

Figure 8.10.4 shows relatively high percolation fluxes, because of the use of the higher infiltration map #2. In most parts of the repository level, the vertical mass fluxes are from 2 to 6 mm/yr, which bound the average surface infiltration of 4.4 mm/yr from infiltration map #2.

Figures 8.10.5 and 8.10.6 show fracture and matrix percolation fluxes, respectively. It is interesting to note that the fracture flow components are very uniform at the repository level, with an average value of 0.4 mm/yr, except for several red spots, indicating lower fluxes. Compared with the fracture flow (Figure 8.10.5), matrix percolation fluxes of Figure 8.10.6 shows a much higher

mass flow, especially along the mountain ridge and at the north-west corner of the model, which correspond to the higher surface infiltration (Figure 8.4.2). The percolation flux through the matrix near the repository ranges from 3 - 8 mm/yr. Also Figures 8.10.6 (dual-k) and 8.10.4 (ECM) show a very similar matrix flow pattern, except that the ECM predictions of higher flux zones are relatively larger in the north-west part of the model domain and along the mountain ridge where infiltration is higher.

A comparison of Figures 8.10.5 and 8.10.6 indicates that at the repository level fracture flow contributes less than 10% of the total percolation flux. This partitioning in matrix and fracture percolation fluxes at the repository level is due to the higher matrix permeability used for the simulations (Figures 8.10.4 to 8.10.6). The matrix permeability used for the repository layer in these simulations is $4.23 \times 10^{-16} \text{ m}^2$ (See Table 8.5.4, parameter set #4, for unit tsw35 for the repository parameters). This high matrix permeability value was estimated by the ITOUGH2 code in order to match the measured liquid saturation profiles layer from the boreholes under the high infiltration rate map #2. Based on the USGS data, the average value of matrix permeability in the TSw at the repository is on an order of $1.0 \times 10^{-18} \text{ m}^2$, which corresponds to a maximum matrix flow of about 0.3 mm/yr. Examination of the other simulation results using parameter sets # 1 to #3 indicates a large variation in the fracture and matrix percolation fluxes at the repository level. The fracture flow percentage varies from 20% to 70% of the total liquid fluxes through the repository.

The matrix permeability is highly variable at the repository areas of the TSw unit. This study shows that the matrix permeability values have significant effects on the partitioning of fracture and matrix flow at the repository level. Different fracture and matrix fluxes at the repository may directly impact the total influx into the drifts and the waste isolation strategy as well. Therefore, further studies are needed for accurately determining the matrix and fracture properties and their spatial distribution around the repository.

8.10.2 Water Recharge Maps at the Water Table

The water recharge maps at the level of the water table are shown in Figures 8.10.7 to 8.10.12. Also in these figures, the unit of mass fluxes of the figures is converted to mm/yr, to compare with the surface infiltration, and "negative" values mean downward flow. The recharge maps at the water table (Figures 8.10.7 to 8.10.12) show a more non-uniform pattern than the repository percolation fluxes, discussed above. This may be due to the much longer flow pathways to the water table than to the repository level, therefore there are more effects of formation heterogeneity on the flow directions.

Figures 8.10.7 and 8.10.8 show a similar recharge map at the water table, even though the percolation fluxes at repository level are quite different (Figures 8.10.1 and 8.10.2). The fast flow pathways to the water table are indicated by the dark blue spots on the two figures.

Figure 8.10.9 shows two higher recharge zones, with 0.4 mm/yr, along the west of the Solitario Canyon fault from south to north, and along the cross section between SD-7, SD-12 and the northern boundary. In the rest of the model domain, very low fluxes (<0.1 mm/yr) are noticed, which are due to lateral diversions for this case.

A much higher recharge rates can be seen in Figure 8.10.10, but the recharge map follows the infiltration pattern (Figure 8.4.2). This indicates that little lateral diversions occur under this modeling scenario.

Vertical Mass Flux at Water Table

Figure 8.10.7

Recharge map at the water table, simulated using the ECM model, parameter set #1 and uniform infiltration rate of 0.1 mm/yr.

Vertical Mass Flux at Water Table

Figure 8.10.8 Recharge map at the water table, simulated using the ECM model, parameter set #2 and uniform infiltration rate of 0.1 mm/yr.

Vertical Mass Flux at Water Table

Figure 8.10.9 Recharge map at the water table, simulated using the ECM model, parameter set #3 and infiltration map #1.

Vertical Mass Flux at Water Table

Figure 8.10.10 Recharge map at the water table, simulated using the ECM model, parameter set #4 and infiltration map #2.

Vertical Fracture Mass Flux at Water Table

Figure 8.10.11 Recharge map at the water table, simulated using the dual-permeability model, parameter set #4 and infiltration map #2.

Vertical Matrix Mass Flux at Water Table

Figure 8.10.12

Recharge map at the water table, simulated using the dual-permeability model, parameter set #4 and infiltration map #2.

Figures 8.10.11 and 8.10.12 show the recharge maps through fracture and matrix for the dual-permeability model, respectively, at the water table. The fracture flow map is very different than the percolation map at the repository level (Figure 8.10.5). As shown in Figure 8.10.11, higher fracture flow fluxes at the water table occur along the major faults, in the eastern part of the model domain. This indicates that fracture flow has been diverted substantially to the east when passing through the CHn unit.

The recharge map through matrix (Figure 8.10.12) shows a good correlation with infiltration map #2 (Figure 8.4.2). This suggests that there is little lateral movement occurring when the water flows through all the unsaturated zones. Also, Figures 8.10.11 and 8.10.12 indicate that fracture flow contributes less than 10% to the total recharge to the water table, i.e., 90% of recharge is from flow through matrix-matrix connections. The two maps in Figures 8.10.10 and 8.10.12 are very similar, and this indicates the ECM and the dual-permeability approaches give similar predictions on water table recharge rates.

8.11 Summary, Conclusions and Recommendations

8.11.1 Summary

A systematic study of 3-D model calibrations and sensitivity analyses is reported in this Chapter. The model calibration efforts summarized in this Chapter were performed using field data on saturation and water potential, gas flow, geothermal condition and heat flow, perched water, and environmental isotopes. The sensitivity studies were conducted to assess the effects of parameter variations, infiltration rate changes, and numerical modeling approaches. Fracture/matrix interactions in welded and unwelded tufts of the unsaturated zone were treated using the generalized ECM and the dual-permeability approach for treating fracture/matrix flow.

In this study, we have conducted a series of three-dimensional modeling simulations to calibrate the 3-D site-scale model to predict the moisture and heat flow and distribution at the Yucca Mountain site. Four sets of rock properties for fracture and matrix, and three sets of properties for faults were used in the model calibration and sensitivity studies. Several three-dimensional models which incorporate the observed moisture and geothermal data were developed. All these models were based on the current 3-D site-scale model grid.

Three different infiltration maps have been incorporated into the site-scale model, which include both uniform and spatially distributed infiltration rates. In addition, we have also conducted a series of sensitivity analysis of the effects of fault and rock properties on lateral and vertical moisture movement through the mountain. The fault properties used in our analyses are derived from pneumatic data analysis, laboratory results for the formation unit, and assumed values.

8.11.2 Conclusions

From the systematic model calibrations and sensitivity analyses of the 3-D, site-scale, unsaturated zone model of Yucca Mountain described in this Chapter, we conclude:

- The moisture distributions predicted by the 3-D model match well with observed water saturation profiles, and are in reasonable agreement with observed water potential data.
- The 3-D model predicted zones of high water saturations at the locations of observed perched water bodies encountered at the boreholes.
- There are significant effects of rock properties and infiltration rates on lateral moisture flow. The PTn unit may divert water thousands of meters laterally toward the east at certain locations at the mountain, depending on the rock properties and infiltration rates used in the simulation. Also large lateral diversions occur around the zeolitic zones in the CHn formation.

Three-Dimensional Model Calibration and Sensitivity Studies

- The controlling factors for the simulated lateral moisture movement in the unsaturated zone are contrasts in capillary pressure forces across interfaces between different grid layers, or capillary barrier effects. The contrasts in capillary forces are affected by heterogeneous rock properties and infiltration rates for given model conditions.
- The three-dimensional saturation distributions simulated by the models at repository horizon are in good agreement with observations from several boreholes.
- The heat flow through the unsaturated zone simulated by the models is also in reasonable match with field measurements.
- Sensitivity studies of three sets of fault properties and associated simulation results indicate that the major faults, as incorporated in the models, act as capillary barriers to lateral flow at low infiltration rates (0.1 mm/yr), and as a conduit or a drain pipe under high infiltration rates of several mm/yr with fault properties used in the studies.
- Lateral flow across faults may occur near the interfaces between the zeolitic units and the TSw or the vitric units, where high water saturated zones are built up in the surrounding zeolitic layers.
- By analyzing water flow down through fractures and matrix from the model results, we could also match the ages of the perched water reasonably well at the locations near boreholes UZ-1/14, and SD-7.
- The dual-permeability and the ECM approaches give almost identical simulation results in terms of predicted matrix and fracture saturations, moisture tensions and total percolation fluxes at the repository horizon under steady-state, three-dimensional flow conditions in the entire site-scale model.
- Percolation fluxes at the repository horizon and recharge maps at the water table are very non-uniformly distributed. They are affected by the surface infiltration rates, heterogeneity of rock property and faults. The predicted repository percolation flux and water table recharge maps indicate that several possible flow pathways may exist.
- The percentage of fracture and matrix flow in the total percolation flux at the repository is highly variable, and is mainly affected by matrix permeability used in the model for the repository horizon formation.

The conclusions above are based on Q data and were obtained from the simulation results using the Q computer codes, TOUGH2, and ITOUGH.

8.11.3 Recommendations

The 3-D model simulations and sensitivity studies reported in this Chapter constitute an important step in understanding fluid and heat flow within the Yucca Mountain. This study provides much confidence in the 3-D site-scale unsaturated zone model for incorporating all the available observed field data and for investigating the mountain's behavior. However, there are still a considerable number of uncertainties in our understanding of the hydrogeological system of Yucca Mountain, especially regarding percolation flux within the mountain. The major uncertainties we are still facing are (1) accuracy in estimated current, past and future net water infiltration rates over the mountain; (2) quantitative description of the heterogeneity in welded and non-welded tuffs, their flow properties and their detailed spatial distributions within the mountain; (3) insufficient field studies, especially on faults and on possible lateral moisture diversion in the PTn formation and in the CHn unit, where the zeolitic zones may play an important role in diverting moisture flow to water table.

Future modeling studies of fluid and heat flow and distribution at Yucca Mountain are advised to focus on (1) incorporating distributed matrix/fracture rock properties; (2) developing updated and accurate geological models for different hydrogeologic units; (3) conducting further comprehensive studies to determine percolation fluxes using field observations of saturation, moisture tension and temperature data, combined with direct and inverse modeling analysis; (4) performing comparative studies of model predictions and field observations regarding percolation fluxes, saturations, and moisture tensions and lateral movement; and (5) investigating effects of faults, thermal loading and air circulation on moisture movement within the mountain.

8.12 References

- Ahlers C.F., C. Shan, C. Haukwa, A.B.J. Cohen, and G.S. Bodvarsson, Calibration and prediction of pneumatic response at Yucca Mountain, Nevada using the unsaturated zone flow model, Yucca Mountain Project Milestone OB12M, 1996.
- Ahlers, C.F., T.M. Bandurraga, G.S. Bodvarsson, G. Chen, S. Finsterle, and Y.S. Wu, Performance analysis of the LBNL/USGS three-dimensional unsaturated zone site-scale model, Yucca Mountain Project Milestone 3GLM105M, Lawrence Berkeley National Laboratory, Berkeley, CA, 1995a.
- Ahlers, C.F., T.M. Bandurraga, G.S. Bodvarsson, G. Chen, S. Finsterle, and Y.S. Wu, Summary of model calibration and sensitivity studies using the LBNL/USGS three-dimensional unsaturated zone site-scale model, Yucca Mountain Project Milestone 3GLM107M, Lawrence Berkeley Laboratory, Berkeley, CA, 1995b.
- ACCN: MOL.19960208.0091-0097
DTN: LB092995312293.001 (Non-Q)

Buesch, D.C., R.W. Spengler, T. C. Moyer, and J.K. Geslin, Revised stratigraphic nomenclature and macroscopic identification of lithostratigraphic units of the Paintbrush Group exposed at Yucca Mountain, Nevada, U.S. Geological Survey Report OFR 94-469, U.S. Geological Survey, Denver, CO, 1995.
DTN: GS931208314211.049 (Q)

DOE, Reference Information Base (RIB), Yucca Mountain Site Characterization Project, 1993

Finsterle, S., ITOUGH2 User's Guide, Version 2.2, Lawrence Berkeley Laboratory, Research Report LBL-34581, UC-600, Lawrence Berkeley Laboratory, Berkeley, CA, 1993.
ACCN: MOL.19941026.0075

Flint, L., Permeability Data for UZ-16 and SD-9, 1995.
DTN: GS950608312231.006

Flint, L.E., and A.L. Flint, Spacial distribution of potential near surface moisture flux at Yucca Mountain, Proceedings of the Fifth International Conference on High Level Radioactive Waste Management, Las Vegas, NV, pp. 2352-58, U.S. Geological Survey, Lakewood, CO, 1995.
DTN: GS940108312212.005 (Non-Q)

Flint, L., Personal communication, 1996.

Flint, A.L., E.L. Flint, and J.A. Hevesi, Conceptual and numerical model of infiltration for the Yucca Mountain area, Nevada, U. S. Geological Survey, Water-Resources Investigation Report-96, Denver, Colorado, 1996.

Fridrich, C.J., W.W. Dudley Jr., and J.S. Stuckless, Hydrogeologic analysis of the unsaturated-zone ground-water system under Yucca Mountain, Nevada, Journal of Hydrology, v. 154, pp.133, 1994.
ACCN: MOL.19940811.0102

Hevesi, J.A., and A.L. Flint, Geostatistical model for estimating precipitation and recharge in the Yucca Mountain Region, Nevada-California, U. S. Geological Survey, Water-Resources Investigation Report, Denver, Colorado, 1995.
DTN: GS960108312111.001 (Non-Q)

Ho, C.K., S.J. Altman, and B.W. Arnold, Alternative Conceptual Models and Codes for Unsaturated Flow in Fractured Tuff: Preliminary Assessments for GWTT-95, Yucca Mountain Site Characterization Project Report, SAND95-1456, September 1995.

Hudson, D.B., and A. L. Flint, Estimation of shallow infiltration and presence of potential fast pathways for shallow infiltration in the Yucca Mountain area, Nevada, U.S. Geological Survey, Water Resources Investigations Report, Denver, CO, 1995 (in review.)
DTN: GS960508312212.006 (Non-Q)

Three-Dimensional Model Calibration and 'Sensitivity Studies

- International Formulation Committee, A formulation of the thermodynamic properties of ordinary water substance, IFC Secretariat, D'Asseldorf, Germany, 1967.
ACCN: NNA.19890918.0501
- Lu, N., and E.M. Kwicklis, A preliminary, two-dimensional numerical model for gas circulation around UZ6s, Yucca Mountain, Nevada, U.S. Geological Survey, Lakewood, CO, 1995.
- Luckey, R.R., Perched water testing - USW SD-7, Personal communication, March, 1995.
- OCRWM/DOE, Technical Data Catalog, Yucca Mountain Site Characterization Project, 1995.
- Oldenburg, C.M., and K. Pruess, On numerical modeling of capillary barriers, *Water Resources Res.*, 29(4), pp. 1045-1055, 1993.
- Pruess, K., TOUGH2 -- a general-purpose numerical simulator for multiphase fluid and heat flow, Lawrence Berkeley Laboratory Report LBL-29400, Lawrence Berkeley Laboratory, Berkeley, CA, 1991.
ACCN: NNA.19940202.0088
- Pruess, K., J.S.Y. Wang, and Y.W. Tsang, On thermohydrologic conditions near high-level nuclear wastes emplaced in partially saturated fractured tuff, Part I. Simulation studies with explicit consideration of fracture effects, *Water Resources Res.*, 26(6), pp.1235-1248, 1990a.
ACCN: NNA.19910328.0073
- Pruess, K., J.S.Y. Wang, and Y.W. Tsang, On the thermohydrologic conditions near high-level nuclear wastes emplaced in partially saturated fractured tuff, part 2. Effective continuum approximation, *Water Resources Res.*, 26(6), pp.1249-1261, 1990b.
- Pruess, K., and T.N. Narasimhan, A practical method for modeling fluid and heat flow in fractured porous media, *Soc. Pet. Eng. J.*, 25, pp. 14-26, 1985.
ACCN: NNA.19910307.0185
- Pruess K., A. Simmons, Y.S. Wu, and G. Mordis, TOUGH2 Software Qualification, Lawrence Berkeley National Laboratory, Berkeley, Ca, February, 1996.
- Pruess, K., GMINC - A mesh generator for flow simulations in fractured reservoirs, Lawrence Berkeley National Laboratory Report LBL-15227, Lawrence Berkeley National Laboratory, Berkeley, California, 1983a.
ACCN: NNA.19910307.0134
- Rousseau J.P., C.L. Loskot, J. Kume, M. Kurzmack, N.D. Brain, K. Thomas, A.J. Greengard, In-situ borehole instrumentation and monitoring data for USW NRG-7a and USW NRG-6, Yucca Mountain, Nye County, Nevada, 1995.

Three-Dimensional Model Calibration and 'Sensitivity Studies

Rousseau, J.P., E.M. Kwicklis, and D.C. Gillies, Hydrogeology of the unsaturated zone, North Ramp Area of the Exploratory Studies Facility, Yucca Mountain, U. S. Geological Survey Water-Resources Investigation, U. S. Geological Survey, Denver, CO, 1996.

Rousseau, J.P., Data transmittal of pneumatic pressure records from 10/24/1994 through 3/31/1996 for boreholes UE-25 UZ#5, USW NRG-6, USW NRG-7a, USW SD-12, and USW UZ-7a, Yucca Mountain, Nevada, U. S. Geological Survey, 1996.

DTN: GS950508312232.004 Q

DTN: GS960308312232.001 Q

Sass, J.H., Lachenbruch, A.H., Dudley, W.W., Jr., Priest, S.S., and Munroe, R.J., Temperature, thermal conductivity, and heat flow near Yucca Mountain, Nevada: some tectonic and hydrologic implications, U.S. Geological Survey Open-File Report 87-649, U.S. Geological Survey, 1988.

ACCN: NNA.19890123.0010

DTN: GS950408318523.001 (Non-Q)

Wilson, M.L., J.H. Gauthier, R.W. Barnard, G.E. Barr, H.A. Dockery, E. Dunn, R.R. Eaton, D.C. Guerin, N. Lu, M.J. Martinez, R. Nilson, C.A. Rautman, T.H. Robey, B. Ross, E.E. Ryder, A.R. Schenker, S.A. Shannon, L.H. Skinner, W.G. Halsey, J.D. Gansemer, L.C. Lewis, A.D. Lamont, I.R. Triay, A. Meijer, and D.E. Morris, Total-system performance assessment for Yucca Mountain - SNL second iteration (TSPA-1993), Sandia National Laboratories Report SAND93-2675, UC-814, Sandia National Laboratories, Albuquerque, NM, 1994.

ACCN: NNA19940112.0123

Wittwer, C., G. Chen, G.S. Bodvarsson, M. Chornack, A. Flint, L. Flint, E. Kwicklis, and R. Spengler, Preliminary development of the LBL/USGS three-dimensional site-scale model of Yucca Mountain, Nevada, Lawrence Berkeley National Laboratory Report LBL-37356, UC-814, Lawrence Berkeley National Laboratory, Berkeley, CA, 1995.

Wittwer, G., G. Chen, and G.S. Bodvarsson, Studies of the role of fault zones on fluid flow using the site-scale numerical model of Yucca Mountain, Proceedings of the Fourth International High Level Radioactive Waste Management Conference, Las Vegas, pp.667-674, 1993.

ACCN: NNA.19931129.0085

DTN: GS930308312293.002 (Non-Q)

Wu, Y. S., S. Finsterle, P. Frazer, and A. Simmons, Software qualification for ITOUGH2 and various equation-of-state (EOS) modules and auxiliary modules for TOUGH2 and ITOUGH2, Report Lawrence Berkeley National Laboratory, Berkeley, CA, August 1996 (draft).

Yang, I. C., G.W. Rattray, and P. Yu, Interpretations of chemical and isotopic data from boreholes in the unsaturated-zone at Yucca Mountain, Nevada, U. S. Geological Survey Water-Resources Investigation Report-96-4058, U. S. Geological Survey, Denver, Colorado, 1996.

TEMPERATURE AND HEAT FLOW ANALYSIS

G. S. Bodvarsson, Y.S. Wu, and S. Finsterle

August 1996

9.1 Introduction

The three-dimensional site-scale model, developed by Lawrence Berkeley National Laboratory (LBNL) in collaboration with the U.S. Geological Survey (USGS), has primarily been used for studies of isothermal moisture movement within the unsaturated zone at Yucca Mountain (Wittwer et al. 1995; Ahlers et al. 1995a; Ahlers et al. 1995b). However, under natural hydrologic and thermal conditions, both liquid and gas (air and vapor) flow in the unsaturated zone of Yucca Mountain is affected by ambient temperature changes, geothermal gradients, atmospheric and water table conditions. Thermal and hydrological regimes are closely related due to the effects of coupling between thermal, density, and atmospheric conditions on air circulation through the mountain (Weeks, 1987; Lu and Kwicklis, 1995).

In addition to effects of natural thermal conditions, heat will also be generated as a result of emplacing high level nuclear waste in the unsaturated zone. The thermal loading from the waste repository will significantly affect the pre- and post waste emplacement performance of the repository. Quantitative evaluation of thermo-hydrologic and thermal loading effects on the performance of the potential high-level nuclear waste repository at Yucca Mountain is essential in conducting site characterization, performance assessment studies, and repository and engineering barrier design. Thus, there is a need to incorporate observed temperature and heat flow data of Yucca Mountain into the three-dimensional, site-scale model in order to enhance the capability for modeling thermal effects.

Sass et al. (1988) examined temperature data from various boreholes at Yucca Mountain. They suggested that the temperature profiles from the boreholes were primarily conductive and did not exhibit a significant convective component. They identified two processes that would explain deviations from conductive behavior. One relates to infiltrating water and the heat consumption caused by the warming of the water as it percolates through the unsaturated zone from the ground surface to the water table. The other involved the possibility of gas flow from deeper areas of the unsaturated zone to shallower areas carrying water vapor that condenses at shallow depths and releases the latent heat. This conceptual model is considered less likely given our current understanding of heat flow properties at Yucca Mountain.

Ahlers et al. (1995) performed conductive heat transfer analysis using the available temperature and heat flow data from the Yucca Mountain site for 25 geologic and hydrologic boreholes (Sass et al., 1988). These temperature logs sug-

gested that geothermal gradients in the unsaturated zone are primarily conductive and range between 15°C/km to 60°C/km. The measured temperature data (Sass et al., 1988), the rock thermal conductivities (Nimick, 1989, 1990; DOE (RIB), 1993; and Rautman, 1995), and the rock thermal capacities (DOE (RIB), 1993) were incorporated into the present three-dimensional site-scale model to simulate thermal effects and to account for the ambient hydro-thermal conditions of the repository. A parameter estimation study was also conducted for calibrating thermal conductivities using an inverse modeling code, ITOUGH2 (Finsterle, 1993) and 1-D submodels. This work is briefly summarized in this chapter.

In the main part of this chapter, we investigate the effects of percolating water from infiltration on the temperature conditions and gradients that exist within the unsaturated zone. Model calculations using ITOUGH2 are used to examine the importance of this process using qualified data from recent boreholes. The results of these analyses are augmented by additional temperature data from non-qualified (non-Q) data from older boreholes (Sass et al. 1988). Finally, summary comments and recommendations are given.

9.2 *QA Status of Data and Software Used in this Chapter*

The temperature data from older boreholes given by Sass et al. (1988) are non qualified (non-Q). Temperature data from boreholes UZ-4, UZ-5, UZ-7a, NRG-6, NRG-7a, and SD-12 are qualified (Q-data) or will be qualified when the data have been submitted to and approved by the Technical Database. Table 9.2.1 gives the appropriate data tracking numbers for the data that are already qualified. The computer software used in this chapter is fully qualified. The ITOUGH2 code qualification is documented in a LBNL report entitled "Software Qualification of ITOUGH2 and various TOUGH2 and ITOUGH2 Equations of State Modules and Auxiliary Modules" by Y.S. Wu, S. Finsterle, P. Fraiser, C.F. Ahlers and A. Simmons (1996).

Table 9.2.1 Qualified temperature data and corresponding data tracking numbers.			
Hole	Investigator	Organization	Data Tracking Number
UZ-4	Rousseau	USGS	9/96: GS960308312232.001
UZ-5	Rousseau	USGS	9/96: GS960308312232.001
UZ-7a	Rousseau	USGS	9/96: GS960308312232.001
NRG-6	Rousseau	USGS	9/96: GS960308312232.001
NRG-7a	Rousseau	USGS	9/96: GS960308312232.001
SD-12	Rousseau	USGS	9/96: GS960308312232.001

9.3 *Temperature and Heat Flow Data*

9.3.1 Temperature Data

Temperature data observed from 35 test boreholes near Yucca Mountain were reported by Sass et al. (1988), and repeated temperature logs were obtained from 18 of these boreholes. We selected 25 boreholes which included all the boreholes with measured temperature data within or near the site-scale model area. The selected borehole location map and the plan view of the model surface area of the site-scale model are shown in Figure 9.3.1, and the coordinates and borehole completion information for the 25 boreholes are given in Table 9.3.1.

Table 9.3.1 also gives the same information for some of the recently drilled boreholes at Yucca Mountain. These include boreholes UZ-4, UZ-5, UZ-7a, NRG-6, NRG-7, and SD-12. The temperature data from these boreholes are qualified (Q data).

The temperature data for most of these boreholes were digitized from the original plots given in the report by Sass et al. (1988). For the recent wells, the temperature data were obtained from J. Rousseau of USGS (see data tracking numbers in Table 9.2.1). Sass et al. (1988) studied these data and concluded that temperature gradients in the unsaturated zone appear primarily conductive and range between 15°C/km to 60°C/km within the study area. Figures 9.3.2-9.3.7 present the observed borehole temperature profiles, showing generally near-linear profiles in the unsaturated zone.

Temperature and Heat Flow Analysis

Table 9.3.1 Location, elevation, and completion information for the selected boreholes					
Source: Yucca Mountain Site Characterization Project, Site Atlas Supplement, October 1993					
	Coordinates		Surface Elevation	Total Depth	Water Level
Boreholes	North (m)	East (m)	(m)	(m)	Depth (m)
UE-25 a#1	-233142	172623	1199	762	469
UE-25 a#4	-234078	172051	1250	152	—
UE-25 a#5	-233768	172137	1236	148	—
UE-25 a#6	-233446	172060	1235	152	—
UE-25 a#7	-233553	172355	1221	305	—
UE-25 b#1	-233246	172644	1201	1220	470
USW G-1	-234848	170993	1325	1829	572
USW G-2	-237386	170842	1554	1831	525
USW G-3	-229447	170226	1480	1533	750
USW G-4	-233418	171627	1270	915	540
USW H-1	-234774	171416	1303	1829	572
USW H-3	-230594	170216	1483	1219	751
USW H-4	-232149	171880	1249	1219	518
USW H-5	-233670	170355	1479	1219	703
USW H-6	-232653	168882	1302	1220	526
USW WT-1	-229801	171828	1202	515	471
USW WT-2	-231849	171274	1301	628	571
UE-25 WT#4	-234242	173139	1167	482	438
UE-25 WT#6	-237920	172067	1313	383	279
USW WT-7	-230298	168826	1197	491	421
USW WT-10	-228225	168646	1123	431	348
UE-25 WT#16	-236043	173856	1210	521	472
UE-25 WT#17	-228118	172581	1124	443	395
UE-25 WT#18	-235052	172168	1336	623	605
USW UZ-1	-235085	170759	1349	387	—
UE-25 UZ#4	-234305	172559	122.5	111.7	—
UE-25 UZ#5	-234267	172558	1204.5	110.6	—
USW UZ-7a	-231845	171397	1288.6	234.2	—
UE-25 NRG-6	-233698	171964	1247.5	335.3	—
UE-25 NRG-7a	-234355	171598	1282.2	461.3	—
USW SD-12	-232244	171177	1323.68	659.6	593.7

Figure 9.3.1

Map of borehole locations used for the conduction study and the study area of the site-scale model.

Figures 9.3.2 - 9.3.3 show the temperature profiles from a series of boreholes UE-25 a#1, a#4, a#5, a#6, a#7 and b#1. Four shallow boreholes of this series, UE-25 a#1, a#4, a#5 and a#7, were drilled within the main drainage of Drill Hole Wash and were believed to have been affected by vertical and lateral movements of fluids. As shown in Figure 9.3.2 - 9.3.3, there exist irregularities and contrasts in thermal gradient that could not be attributed to heat conduction and may be associated with convection heat transfer by vertical and lateral movements of fluids within the upper part of the unsaturated zone in Drill Hole Wash. Borehole UE-25 b#1 (Figure 9.3.3) is near the main surface drainage of Drill Hole Wash, and also shows some degree of disturbance to the temperature field in the unsaturated zone. Between 300 - 600 m elevation, which is below the water table, the profile is nearly isothermal and suggests that very strong

Figure 9.3.2
Observed temperature profiles for UE-25: a#1, a#4 and a#5. Data from Sass et al. (1988).

Figure 9.3.3
Observed temperature profiles for UE-25: a#6, a#7 and b#. Data from Sass et al. (1988).

heat convection is occurring. Below 200 m elevation, the profile is linear with a gradient of about $23^{\circ}\text{C}/\text{km}$, suggesting conductive heat flow. It should be noted that the water table is located at an elevation of approximately 730 meters above sea level for most of the boreholes considered.

The temperature profiles from the "G" series boreholes, USW G-1, G-2, G-3 and G-4, are shown in Figure 9.3.4. These boreholes were drilled primarily to obtain geologic data, although considerable hydrologic and thermal information has been obtained from them. The temperature profile for G-2 shows downflow at elevations between 900-700 m.a.s.l., and this has been analyzed by Czarnecki et al. (1994) and Sass (1996).

Figure 9.3.4
Observed temperature profiles for G-series boreholes, USW G-1, G-2, G-3 and G-4. Data from Sass et al. (1988).

Figure 9.3.5
Observed temperature profiles for H-series boreholes, USW H-1, H-2, H-3 and H-4. Data from Sass et al. (1988).

Figure 9.3.5 shows the temperature profiles from the "H" series boreholes, USW H-1, H-3, H-4, H-5, and H-6. These boreholes were drilled primarily for hydrologic studies. The temperature behavior is similar to that of the "G" series.

Figure 9.3.6
Observed temperature profiles for USW UZ-1, WT-1, WT-2, WT#4 and WT#6. Data from Sass et al. (1988).

Figure 9.3.7
Observed temperature profiles for USW WT-7, WT-10, WT#16, WT#17 and WT#18. Data from Sass et al. (1988).

Figures 9.3.6 and 9.3.7 present the measured temperatures for the "WT" series and UZ-1 holes. These boreholes are primarily for engineering studies of the unsaturated zone and water table. The thermal gradients, as shown in Figures 9.3.6 and 9.3.7, vary from about 20°C/km to 60°C/km in the unsaturated zone.

Figure 9.3.8

Observed temperature profiles for UZ-4, UZ-5, UZ-7a, SD-12, NRG-6 and NRG-7a. Data from Rousseau et al. (1996) and unpublished data by Rousseau of USGS.

Figure 9.3.8 shows the measured stable temperatures in boreholes UZ-4, UZ-5, UZ-7a, NRG-6, NRG-7 and SD-12. These temperature data are generally much more accurate than those from Sass et al. (1988) because these holes were instrumented with long term monitoring equipment. The data reported in Sass et al. (1988) were measured in gas filled or liquid filled boreholes. This can very significantly affect the temperature measurements in various ways primarily due to internal well flows. The data shown in figure 9.3.8 are, however, similar to the rest of the holes. This provides some indication that the data in Sass et al. (1988) are of sufficient quality to generate useful scientific, although not qualified conclusions.

9.3.2 Heat Flow Data

Sass et al. (1988) estimated the conductive heat flow at the Yucca Mountain site based on the temperature surveys and thermal conductivity measurement in both the saturated and the unsaturated zones. They found that heat flows in the unsaturated zone vary in a systematic fashion, both geographically and as a function of the unsaturated zone thickness. The average heat flow from the unsaturated zone is about 41 mW/m^2 (see Figure 9.3.9). In comparison, the limited temperature data available for the saturated zone indicates an average heat flux of some 50 mW/m^2 (Sass et al., 1988; Rousseau et al., 1996).

Temperature and Heat Flow Analysis

The site-scale model study area is near the southern boundary of a regional heat flow anomaly, the Eureka Low. As indicated by Sass et al. (1988), average heat flow in the Eureka Low is about half that for the adjacent regions. Fridrich et al. (1994) suggests two related interpretations for the heat flow anomaly under Yucca Mountain. First, part of the anomaly results from cool underflow in the deep carbonate aquifer. Second, the correspondence of the northern limit of the heat-flow anomaly to the steep potentiometric gradient to the north suggests that the effective northern limit of the deep carbonate aquifer, and by inference, the zone of downwelling fluid, may coincide with the large lateral potentiometric gradient under Yucca Mountain. The heat flow values within the general site scale model domain range between about 35–45 mW/m², as shown in Figure 9.3.9. The contours of the figure show low heat flow in the central portion and increasing heat flow away from the center of the site-scale model area. It should be noted that the data shown in Figure 9.3.9 do not include qualified data from the recently drilled boreholes.

9.4 *Heat Conduction Analysis*

9.4.1 Model Description

In the heat conduction analysis of the temperature data, we only use the borehole data from Sass et al. (1988). At the time this work was performed, LBNL had not received the more recent qualified temperature data. The data from Sass et al. (1988) are sufficient for the intended use of this analysis which is to investigate to what extent heat conduction can explain the available data. The next section of this chapter investigates how a combined convection/conduction analysis fits all of the available data.

At the locations of the 25 boreholes used in this work, we extracted the appropriate 1-dimensional columns from the UZ model. These columns contain the proper geological information including layering, dipping, and other data. They also contain the correct ground surface elevations (topography) and the location of the water table.

9.4.2 Model Parameters And Boundary Conditions

Model parameter specifications, rock properties and boundary conditions were specified following the framework of the site-scale model (Wittwer et al., 1995; Ahlers et al., 1995). The additional parameters and conditions for simulating thermal effects are presented in this section. Spatially varying constant temperatures were specified at the bottom of the model. The temperature values were taken and interpolated from the borehole temperature data reported by Sass et al. (1988).

Constant temperatures at the upper model boundary (ground surface) were specified with an averaged value of about 18°C, which was derived from extrapolation of the shallow temperature data to the ground surface.

Porosity, rock grain density, thermal conductivities, and rock specific heat used in the model are described in Ahlers et al. (1995).

We have also used a thermal conductivity model, recently developed by Rautman (1995a, 1995b). This model correlates thermal conductivity as a function of porosity, temperature and saturation at the Yucca Mountain site. Thermal conductivity is one of the key heat transfer properties and a controlling factor for conductive heat flow around the repository area. In an effort to look at the response and sensitivity of the model temperature fields to the thermal conductivity data, and to best estimate the thermal conductivity values for the different rock types, we have performed a parameter estimation study using the inverse modeling code, ITOUGH2 (Finsterle, 1993). The ITOUGH2 code solves the inversion problem of a TOUGH2 simulation to estimate model parameters by an automatic model calibration and optimization procedure. The ITOUGH2 simulations were carried out using the observed temperature logs of the selected 25 boreholes to identify and estimate an optimum thermal conductivity set for the site-scale model. As discussed in Chapter 4 (Wu et al.) and in an

accompanying software QA document (Wu et al., 1996), the ITOUGH2 code is qualified.

9.4.3 Simulation And Comparison

The measured temperature data were compared with the three-dimensional simulation results for boreholes within and near the model area. For rock thermal conductivities, the tabulated data in RIB, Rautman's model (1995b), and ITOUGH2 (optimized) values were used in the simulations. The simulated temperature profiles are plotted for boreholes H-3 and H-5 in Figures 9.4.1 and 9.4.2, as dashed, solid and dotted curves for RIB, Rautman's model, and the ITOUGH2 estimated (Fitted) parameters, respectively. The observed temperature data are represented by symbols in the figures with the logging dates specified. These plots just show examples of the matches obtained; the reader is referred to Ahlers et al. (1995) for detailed descriptions of all of the matches with the available borehole temperature data.

Figure 9.4.1
Comparison between measured temperature data for well H-3 (Sass et al., 1988) and various ITOUGH2 optimized profiles.

Figure 9.4.2
Comparison between measured temperature data for well H-5 (Sass et al., 1988) and various ITOUGH2 optimized profiles.

Figure 9.4.3 shows observed temperature data for borehole H-3 and calculated values for comparison. It is clear that all of the thermal conductivity models match the data reasonably well, but the Rautman thermal conductivity model does the best. This was actually the case for most of the borehole data

(Ahlers et al., 1995). The rather steep temperature gradient in the Topopah Springs Unit (elevation between 1350 and 1100 m.a.s.l.) is matched by ITOUGH2 using heat thermal conductivities than the values measured. As suggested in the next section, conductive heat transfer cannot fully explain the observed temperature data for many boreholes at Yucca Mountain, perhaps because of a significant amount of water percolating through the unsaturated zone and absorbing some of the heat flux rising from depth.

Figure 9.4.2 shows another example. In this case, we examine borehole H-5, which is located close to the crest of Yucca Mountain, as is the previous borehole, H-3 (see Figures 9.3.1 and 9.5.1). The temperature data from this borehole are also matched reasonably well by the ITOUGH2 conductivity model. A close examination shows that the rather low gradient in temperature in the Topopah Spring Unit is not well matched, perhaps again due to the lack of percolating water in the model used. Temperature in deeper formations show some scatter, perhaps due to measurement errors.

In general, almost all of the temperature data from the 25 boreholes selected from Sass et al. (1988) are matched reasonably well with the conduction-only model. Certain features as derived above are not really explained by such a model and perhaps require a more general conduction/convection model developed in the next section. However, there is also uncertainty about the quality of temperature data from gas and liquid filled boreholes.

9.5 *Analysis of Temperature Data Using a Coupled Conduction/Convection Model*

The heat conduction analysis performed in the last section did reasonably well in explaining the trends of the temperature data but there were still some significant differences. For many of the wells, the observed temperature gradient in some of the units including Topopah Springs and Calico Hills were less than that obtained by the model. The ITOUGH2 code tried to obtain better matches by increasing thermal conductivities, thereby allowing for the same heat flux using a smaller temperature gradient. As thermal conductivity data are fairly accurate one does not expect that significant errors in thermal conductivity or spatial variability of thermal conductivity exists within the units. An alternative explanation for these smaller temperature gradients is percolating water through the unsaturated zone. In order for this water to increase in temperature from the average surface temperature of 19°C to temperatures around 30°C, some energy must be utilized. Significant downflow percolation will affect the temperature gradients within the unsaturated zone considerably, as pointed out by Sass et al. (1988) and Rousseau et al. (1996).

The percolation flux through the unsaturated zone is believed to be the most important parameter for performance assessment and TSPA calculations

for the Yucca Mountain site. The percolation flux affects the amount of flow into drifts, the number of canisters that may be affected, the waste mobilization issue, and the transport of the radionuclides to the water table. As the spatial and temporal variability of the percolation flux is difficult to measure directly, it must be determined or bounded by indirect methods such as modeling of moisture tension, saturation, and environmental isotope data. If temperature data can be of use in determining or bounding the value of percolation flux, this would be of great importance, and much needed. In the following analysis we start by using the available qualified temperature data to investigate the percolation flux and then proceed to add non-qualified data as collaborative evidence.

9.5.1 Percolation Flux Analysis Using Qualified Temperature Data

The boreholes with qualified temperature data include UZ-4, UZ-5, UZ-7a, NRG-6, NRG-7a, and SD-12. The data from these boreholes were collected by J. Rousseau and others at USGS (see data tracking numbers from Table 9.2.1). The temperature data from these boreholes are of very good quality as the boreholes were instrumented with long term monitoring equipment. The temperature data are shown to be relatively stable and should accurately reflect the actual temperature conditions within the unsaturated zone. Figure 9.3.8 shows all of the temperature data and indicates that most of the boreholes extend only to shallow regions of the unsaturated zone. The only borehole that goes entirely through the TSw is borehole SD-12. The rest of the boreholes basically go through the Paintbrush Unit and perhaps just to the top part of the Topopah Springs Unit. However, the data from boreholes UZ-7a, NRG-6, NRG-7a and SD-12 allow for reasonable determination of the temperature gradient within the Topopah Springs Unit. The values obtained are about 17°C per kilometer for boreholes UZ-7a and SD-12, and about 21°C per kilometer for boreholes NRG-6 and NRG-7a.

In order to convert temperature gradients into estimates of percolation flux, one must assume a conceptual model. A reasonable model is one that assumes that the heat flux E through the unsaturated zone is the sum of the conductive upward heat flow and the downward energy flux due to percolating water. In this case the following equation can be derived:

$$E = \lambda \cdot \nabla T - q_l \cdot \rho_l \cdot c_l \cdot \Delta T \quad (9.5.1)$$

Here, $\lambda = 1.73 \text{ W/m/}^\circ\text{C}$ is heat conductivity, q_l is the volumetric liquid flow rate, $\rho_l = 1000 \text{ kg/m}^3$ is water density, $c_l = 4187 \text{ J/kg/}^\circ\text{C}$ is the specific heat of liquid water, $\Delta T = 14^\circ\text{C}$ is the temperature change the downwardly percolating water undergoes as it moves from the surface to the water table.

The above values for the thermal conductivity and the water density and specific heat are reasonable averages from measurements on cores (data on thermal conductivity taken from RIB; DOE 1993) and from the equation of state for water.

In order to calculate the percolation flux (q_1), one needs an estimate for the average heat flux E through the region penetrated by the above boreholes. Sass et al. (1988) reviewed all of the data available at that time and concluded that the heat flux through the unsaturated zone varied from 30-60 mW/m² (see Section 9.3.2). When they used the temperature data from the unsaturated zone, they obtained values around 41 mW/m². However, it should be noted that this heat flux is derived from temperature gradients in the Topopah Springs assuming only conduction and neglecting the convective component. Sass et al. (1988) also estimated the heat flux from temperature data taken from the saturated zone and arrived at an average value of some 50 mW/m². As this estimate is independent of the unsaturated zone temperature gradient, it may be more reasonable for our analysis of percolation flux.

If one uses a heat flux of $E=50$ mW/m² (in equation 9.6.1), one can derive a percolation flux of about 10 mm/yr for the areas around boreholes SD-12 and UZ-7a, and a percolation flux of about 7 mm/yr for areas around boreholes NRG-6 and NRG-7a. These are fairly large percolation flux values, but they agree reasonable well with the range of infiltration values given by A. Flint in his latest infiltration map (Flint et al., 1996). They present infiltration values that range from almost no infiltration rate to about 12 mm/yr. Flint et al. (1996) estimate an average infiltration rate in the repository area of some 4-5 m/yr based on 8 years of monitoring data. These estimates therefore represent infiltration values for the current climate. If one assumes that heat flux through the unsaturated zone is 40 mW/m², one can calculate an effective percolation flux of 6 mm/yr for the area around SD-21 and UZ-7a, and 2 mm/yr for boreholes NRG-6 and NRG-7a. Again, these are values that are in the range of the infiltration rates estimated by Flint et al. (1996). Also, temperature analysis of shallow boreholes UZ-4 and UZ-5 performed by Rousseau et al. (1996) show infiltration rates of 5-15 mm/yr which is consistent with the above analysis and results.

In summary, all of the temperature data from the recently drilled boreholes, UZ-4, UZ-5, UZ-7a, NRG-6, NRG-7a, and SD-12 indicate very significant percolation of water through the unsaturated zone at Yucca Mountain. Given the importance of the percolation flux parameter, these results are very significant and should be verified by further temperature measurements and other indirect analysis. They should also be verified using the full three-dimensional UZ model.

9.5.2 Percolation Flux Analysis Using Non-Qualified and Qualified Temperature Data

Similar analysis to the one performed in the last section can be done using both qualified and non-qualified data. In addition to the 7 boreholes that have qualified data, we use the additional 25 boreholes from Sass et al. (1988) that have non-qualified data. The borehole locations used in the analysis are shown on the topographic map in Figure 9.5.1. This figure shows that most of the boreholes are located in washes and very few along ridge tops. The data from these boreholes may therefore be biased and not representative of the average conditions within the mountain. The approach taken was to estimate the

Figure 9.5.1

Locations of boreholes used in the coupled convection/conduction analysis superimposed on an elevation contour map.

temperature gradients in the Topopah Springs Unit for all of the boreholes and contour the results as shown in Figure 9.5.2.

The figure shows remarkably consistent patterns with large areas within the unsaturated zone where similar temperature gradients are found. The lowest temperature gradients are found along the crest of Yucca Mountain and towards the Ghost Dance Fault. These temperature gradients are on the order of 16-18 °C per kilometer. Another area with similar low temperature gradients is found in the vicinity of boreholes UZ-1, G-1, H-1 and UT-18. Almost the entire repository region is estimated to have a low temperature gradient in the Topopah Springs unit thereby suggesting a fairly large percolation flux on the order of 5-12 mm/yr depending upon the assumed geothermal heat flux. In the area between the Ghost Dance Fault and the Bow Ridge Fault considerably higher temperature gradients are found, generally increasing towards Bow Ridge Fault. The estimated percolation fluxes in this area are in the neighborhood of some 0-6 mm/yr, but this again depends on the assumed heat flux through the unsaturated zone. It should be noted that the contour map shown in Figure 9.5.2 is very approximate and ignores major structural features. One may argue that the main low temperature gradient area in Figure 9.5.2 should extend between the Solitario Canyon fault and the Calico Hills fault.

Figure 9.5.2

Temperature gradient contour map for the Topopah Springs Unit based on qualified and non-qualified temperature data for the boreholes shown. The temperature data were collected by Sass et al. (1988) and Rousseau et al. (1996).

The above analysis and the temperature gradient data shown in Figure 9.5.2 are in some agreement with the latest infiltration map prepared by A. Flint et al. (1996). Flint et al. (1996) estimated the largest infiltration rate at the crest of Yucca Mountain with different degrees of reductions towards the east and the west. Their zone of large infiltration is much thinner areally than the one suggested by the data in Figure 9.5.2., but one must remember that direct comparison between infiltration rates at the ground surface and percolation flux at the repository region is not possible. We must also note that variable infiltration between areas of sideslope areas with thick alluvium and areas on top of ridges is not considered here. Most of the wells in the present analysis are located in or near washes and these may have substantially different average infiltration and percolation than the entire area considering all surface process and features (see Figure 9.5.1). Flint et al. (1996) conclude that most infiltration occurs near crests and sideslopes whereas the temperature analysis by Rousseau et al. (1996) suggests highest infiltration in channels of washes. It is therefore not clear if the present estimates for percolation flux may be high or low for the entire repository region.

Figure 9.5.3

Spatial distribution of percolation flux at the repository horizon using Flint et al. (1996) infiltration map. (Figure is taken from Chapter 8, Wu et al.).

A useful insight may be gained from the 3-D simulations presented in Chapter 8 (Wu et al., 1996). Figure 9.5.3 shows the computed percolation flux at the repository level using the latest infiltration map by Flint et al. (1996) and the latest matrix and fracture properties given in Chapter 3 (Bandurraga et al., 1996). Comparison between Figures 9.5.2 and 9.5.3 shows that they are very similar in terms of areas of high and low percolation fluxes. If we were to assume an average heat flux of about 45 mW/m^2 , the average value between the heat flux for the saturated zone and the unsaturated zone, the numerical values in both flux maps of Figures 9.5.2 and 9.5.3 would be very similar. We conclude that the average flux through the repository in the TSw is on the order of 5 mm/yr .

Although there are definite trends in the temperature gradients as shown in Figure 9.5.2, there is one borehole that exhibits an interesting temperature profile. Borehole UZ-7a is drilled through the Ghost Dance Fault and actually resides within the fault for hundreds of meters. This borehole only penetrates about 120 meters of the Topopah Springs units. Temperature data from this borehole has been measured by J. Rousseau of USGS. A temperature gradient of about 18°C/km is found in the bottom 50 meters of the borehole and this gradient is given in Figure 9.5.2. This temperature gradient is found below the elevation at which the borehole exits the Ghost Dance Fault. In the top 70 meters of the Topopah Spring, where the borehole resides within the fault zone, a tem-

perature gradient of about $26^{\circ}\text{C}/\text{km}$ is measured. If these temperature gradients are used in equation 9.5.1, one obtains about $1\text{ mm}/\text{yr}$ percolation through the Ghost Dance Fault, but on the order of $5\text{ mm}/\text{yr}$ in the rock mass adjacent to the fault. However, this analysis of the data may be in error because of the very limited available data set. For example, it can be argued that temperature gradients in the top 100 meters of a unit are not reliable as they reflect temperatures and gradients of the adjacent unit, especially if the thermal conductivities of the two units are quite different, which is the case with the Paintbrush unit and the Topopah Springs unit.

9.6.3 Percolation Flux Through the Calico Hills Using Non- Qualified Data

Similar analysis was performed using the temperature data from the Calico Hills Unit. Only the non-qualified data were used since very limited qualified temperature data are available. Again, we use the 25 boreholes from Sass et al. (1988). Figure 9.5.4 shows the temperature gradient in the Calico Hills in the region of interest. The figure shows that the temperature gradient in the Calico Hills is much larger than that of the Topopah Springs Unit because of the much lower effective thermal conductivity of the Calico Hills Unit. The temperature gradients in the Calico Hills Unit vary from about 28 to over $40^{\circ}\text{C}/\text{km}$. There is one anomalous temperature gradient value of $24^{\circ}\text{C}/\text{km}$ for borehole H-3 and another one of $38^{\circ}\text{C}/\text{km}$ for borehole H-1. The thermal conductivity of the Calico Hills Unit varies considerably depending on the vitric or zeolitic nature of the formation as well as the degree of welding and the degree of water saturation. A relatively low effective thermal conductivity estimate would be $1.2\text{ W}/\text{m}^{\circ}\text{C}$ (RIB; DOE 1993). If this value is adopted and heat flux of $50\text{ mW}/\text{m}^2$ is assumed, one can calculate a percolation flux of $7\text{ mm}/\text{yr}$ through most of the Calico Hills Unit. If the same value of thermal conductivity is assumed and a heat flux of $40\text{ mW}/\text{m}^2$ is used, an effective percolation flux of about $2\text{ mm}/\text{yr}$ can be computed. In general, the low temperature gradient area basically covers the entire repository area.

Figure 9.5.4

Approximate temperature gradient contour map for the Calico Hills Unit based on qualified and non-qualified temperature data for the boreholes shown. Temperature data were taken from Sass et al. (1988).

It is interesting to note that although the above percolation flux values are quite substantial, they are less than those estimated through the TSw. One possible explanation of this is lateral flow on top of the zeolites in the CHn as hypothesized in our conceptual model discussion in Chapter 1 (Bodvarsson et al., 1996). The suggested lateral flow above the zeolite is an important conceptualization because of the potential for retardation if the water actually flows through the zeolitic rock (Robinson et al., 1995). Other supporting evidence for this is the fact that H-3 has the lowest temperature gradient in the CHn, and H-3 is close to the region where there is a hole in the zeolites of the CHn, therefore allowing fluid to percolate freely through the unit (see Chapter 1; Bodvarsson, et al., 1996). Also, borehole H-1 has the highest temperature gradient and this borehole only has zeolitic rocks in the Calico Hills unit.

9.6.4 Combined Numerical Analysis of Temperature Gradients in TSw and CHn Using Both Qualified and Non-Qualified Data

The ITOUGH2 computer code was used to estimate percolation flux using all of the temperature data from the 7 qualified wells and the 25 boreholes from Sass et al. (1988). In these simulations, the thermal conductivities of all units were fixed using the values discussed in Ahlers et al. (1995), but the infiltration flux at the ground surface and the percolation flux through the units were estimated. The results showed very comparable percolation flux values to what can be inferred from Figure 9.5.3 and 9.5.4 when the data in these figure are averaged. Since these simulations were conducted using a 1-dimensional model for each one of the boreholes, the infiltration rate at the top, the percolation flux through TSw and the percolation flux through CHn were all assumed to be equal. As Figures 9.5.2 and 9.5.3 and the analysis above have shown, the percolation flux through the TSw seems to be higher than that through the CHn due to lateral flow perhaps around the zeolitic zones. The ITOUGH matches with the data therefore represent an average percolation flux for the two units and probably do not reflect the actual, more complex 2-D and 3-D flow patterns within the unsaturated zone.

Further analysis will be conducted during FY97 that will consist of ITOUGH2 temperature inversions above the CHn using temperature data from all units and then a separate analysis for temperature inversion within the CHn. These analyses will also take into account in more detail the different thermal conductivity variations within all units of the unsaturated zone. Then the results will be applied to the entire 3-D model and the temperature data and gradients from all of the boreholes will be matched simultaneously.

9.7 Concluding Remarks

Lawrence Berkeley National Laboratory (LBNL), in cooperation with USGS, is developing and enhancing the three-dimensional site-scale numerical model of the unsaturated zone at Yucca Mountain. In this chapter, preliminary work on incorporating temperature and thermal conditions into the model is described.

Qualified temperature data from seven boreholes and non-qualified data from twenty-five boreholes are used. Conduction analysis of the data show good matches with temperatures for most of the boreholes and that the thermal conductivity model by Rautman et al. (1995) best explains the data (Ahlers et al., 1995). ITOUGH2 optimization of thermal conductivities generally tends to increase values to obtain a smaller temperature gradient within the Topopah Springs Unit. This is believed to be an artifact of the conduction-only model used as water percolating through the mountain affects the temperature gradient. All of the above conclusions are non-qualified (non-Q) but are believed to be scientifically valid.

A coupled convection/conduction model was also used to analyze the temperature data, and in particular for the purpose of estimating the percolation flux through the mountain. Qualified data from boreholes UZ-7a and SD-12 suggest a percolation flux of some 5 to 10 mm/yr depending upon the assumed heat flux. Qualified data from boreholes NRG-6 and NRG-7a suggest percolation flux of around 2-6 mm/yr, again depending upon the assumed heat flux. These percolation flux values are in reasonable agreement with the recently developed infiltration map (Flint et al., 1996).

The qualified data set from the seven boreholes is augmented by twenty-five non-qualified temperature profiles from boreholes predicted by Sass et al. (1988). The coupled conduction/convection model was applied to all of the available data in order to develop an appropriate percolation map for the proposed repository region. The results show that there are very consistent trends in the temperature gradient data throughout the mountain. Assuming reasonable heat flux values one obtains a percolation flux through the repository horizon in the Topopah Springs Unit of some 5 to 10 mm/yr. We believe that the flux is probably closer to 5 mm/yr given the nature of the assumptions and approximations used. These results are consistent with the computer generated percolation flux map of the repository horizon that results from three-dimensional numerical simulations using the unsaturated-zone model. Analysis of temperatures of the Calico Hills and deeper units show, in general, less of a percolation flux, suggesting lateral flow above the unit, perhaps due to the low permeability zeolites.

It should be emphasized that the analysis presented here is preliminary and needs to be verified by a careful selection of thermal conductivities and heat flow, and a more realistic model. Alternative processes that can explain the temperature data, such as vapor condensation, should be evaluated.

9.8 References

- Ahlers C.F., T.M. Bandurraga, G.S. Bodvarsson, G. Chen, S. Finsterle, and Y.S. Wu, Performance analysis of the LBNL/USGS three-dimensional unsaturated zone site-scale model, Lawrence Berkeley National Laboratory, 1995a.
- Ahlers C.F., T.M. Bandurraga, G.S. Bodvarsson, G. Chen, S. Finsterle, and Y.S. Wu, Summary of model calibration and sensitivity studies using the LBNL/USGS three-dimensional unsaturated zone site-scale model, Lawrence Berkeley National Laboratory, 1995b.
ACCN: MOL.19960208.0091-0097
DTN: LB092995312293.001

Temperature and Heat Flow Analysis

- Czarnecki J.B., G.M. O'Brien, P.H. Nelson, Is there Perched Water Under Yucca Mountain in borehole USW G2?, EOS, Transactions, American Geophysical Union, 1994 Fall Meeting, Vol.75, NO.44, Supplement, November, 1994
ACCN: MOL.19950131.0438
- DOE, Reference Information Base (RIB), Yucca Mountain Site Characterization Project, 1993
- Finsterle S., ITOUGH2 User's Guide Version 2.2, Lawrence Berkeley National Laboratory Report LBNL-34581, Lawrence Berkeley National Laboratory, Berkeley, CA, 1993.
ACCN: MOL.19941026.0075
- Flint A.L., J.A. Hevesi, and L.E. Flint, Conceptual and numerical model of infiltration for the Yucca Mountain area, Nevada, U. S. Geological Survey Water Resources Investigation Report, U. S. Geological Survey, Denver, CO, 1996.
- Fridrich C.J., Dudley, W.W., Jr., and Stuckless, J.S., Hydrogeologic analysis of the unsaturated-zone ground-water system under Yucca Mountain, Nevada, Journal of Hydrology, V. 154, p.133, 1994.
- Lu N, and E. M. Kwicklis, A preliminary, two-dimensional numerical model for gas circulation around UZ6s, Yucca Mountain, Nevada, U.S. Geological Survey, Lakewood, CO, 1995.
- Nimick F. B., Thermal-conductivity data for tuffs from the unsaturated zone at Yucca Mountain, Nevada, Sandia National Laboratory Report SAND88-0642, UC-70, Sandia National Laboratory, Albuquerque, NM, 1989.
ACCN: NNA.19900328.0105
- Nimick F. B., The thermal conductivity of seven thermal/mechanical units at Yucca Mountain, Nevada, Sandia National Laboratory Report, SAND88-1387, UC-814, Sandia National Laboratory, Albuquerque, NM, 1990.
ACCN: NNA.19891107.0078
- Rautman C.A., Modeling spatial heterogeneity of thermal conductivity using a surrogate property, Proceedings of the Sixth Annual International Conference on High-Level Radioactive Waste Management, Las Vegas, NV, pp.83-84, 1995a.
ACCN: MOL.19950321.0080
- Rautman C.A., Preliminary geostatistical modeling of thermal conductivity for a cross section of Yucca Mountain, Nevada, Sandia National Laboratory Report, SAND 94-2283, WC-814, Sandia National Laboratory, Albuquerque, NM, 1995b.
DTN: SNSAND94228300.000 (Non-Q)
- Robinson B.A., A.V. Wolfsberg, G.A. Zyvoloski, and C.W. Gable, An unsaturated zone flow and transport model of Yucca Mountain, LA-Milestone 3468 (Draft), 1995.

Temperature and Heat Flow Analysis

- Rousseau J.P., E.M. Kwicklis, and D.C. Gillies, Hydrogeology of the unsaturated zone, North Ramp Area of the Exploratory Studies Facility, Yucca Mountain, U. S. Geological Survey Water-Resources Investigation, U. S. Geological Survey, Denver, CO, 1996.
- Sass J.H., Significance of the temperature profile in USW-G2 and its evolution with time, manuscript in prep, update May, 1996.
- Sass J.H., Lachenbruch, A.H., Dudley, W.W., Jr., Priest, S.S., and Munroe, R.J., Temperature, thermal conductivity, and heat flow near Yucca Mountain, Nevada: some tectonic and hydrologic implications, U.S. Geological Survey Open-File Report 87-649, U.S. Geological Survey, 1988.
ACCN: NNA.19890123.0010
DTN: GS950408318523.001 (Non-Q)
- Weeks E.P., Effect of topography on gas flow in unsaturated fractured rock: concepts and observations, flow and transport through unsaturated fractured rock, (D.D. Evans and T.J. Nicholson, Eds.), Geophysical Monograph 42, American Geophysical Union, Washington, D.C., pp.165-170, 1987.
ACCN: HQS.19880517.3214
- Wittwer C., G. Chen, G.S. Bodvarsson, M. Chornack, A. Flint, L. Flint, E. Kwicklis, and R. Spengler, Preliminary development of the LBL/USGS three-dimensional site-scale model of Yucca Mountain, Nevada, Lawrence Berkeley National Laboratory Report LBL-37356, UC-814, Lawrence Berkeley National Laboratory, Berkeley, CA, 1995.
- Wu. Y.S., S. Finsterle, P. Frazer, and A. Simmons, Software qualification for ITOUGH2 and various equation-of-state (EOS) modules and auxiliary modules for TOUGH2 and ITOUGH2, Report Lawrence Berkeley National Laboratory, Berkeley, CA, August 1996 (draft).

**PRELIMINARY CONCEPTUAL MODEL
OF FLOW PATHWAYS
BASED ON ^{36}Cl AND OTHER
ENVIRONMENTAL ISOTOPES**

J. Fairley and E. Sonnenthal

August 1996

10.1 Introduction

Environmental isotopes are stable isotopes that are produced either in the atmosphere, in surface and ground waters, or *in situ* in rock, soil, and alluvium. Examples of commonly used environmental isotopes are deuterium (^2H), ^3H , ^{14}C , ^{18}O , and ^{34}S . Some of the more exotic environmental isotopes involve ^3He and other noble gases. Because environmental isotopes fractionate in nature, their concentrations change as a function of temperature, pressure, and source region. The concentrations of environmental isotopes relative to their background ratios can therefore be utilized to obtain information about source regions, climatic conditions, mixing of different reservoirs, and residence time in a particular reservoir. A special class of environmental isotope tracer includes those from anthropogenic sources (i.e., nuclear testing), such as ^{36}Cl , ^{129}I , ^3H , ^{99}Tc , ^{243}Pu , and ^{137}Cs . As tracers these have been useful in evaluating flow pathways from the surface through the unsaturated zone at Yucca Mountain. Because of their occurrence at Yucca Mountain, ^{36}Cl and ^3H concentrations, in particular, provide important insights into fast pathways in the unsaturated zone.

Although environmental isotopes are very good tracers of pathways, past events, and indicators of residence times in rock or water, they have limitations. A common misconception is that concentrations of environmental isotopes can be used to determine percolation flux to the horizon where they are found. For example, they can show that a pulse of water deposited material in a fracture lining at some period in time, but not how much water passed that location. Furthermore, the mere detection of a tracer such as ^{36}Cl at repository depth tells nothing about the significance of its occurrence in a performance sense, i.e., the level of concentration of the isotope that would lead to estimates of detrimental performance with respect to flow pathways. Nonetheless, in spite of their limitations, environmental isotopes provide a useful tool for calibration of the site-scale unsaturated zone flow model because they provide an additional line of evidence for testing consistency of conceptual and numerical models with observations. It is for the purpose of model calibration that we discuss issues related to environmental isotopes with emphasis on their confirmation of fast flow pathways through the unsaturated zone.

10.1.1 ^{36}Cl : Measurements, Assumptions, Caveats

^{36}Cl is produced by a number of sources which can be grouped into atmospheric sources and *in situ* production. Atmospheric sources include natural sources and anthropogenic sources, such as global fallout and local Nevada Test Site (NTS) activities. ^{36}Cl is produced naturally in the atmosphere by reaction of

cosmic rays with ^{40}Ar , ^{36}Ar , and ^{36}Cl . ^{36}Cl has a half-life of 308,000 years and residence time in the stratosphere on the order of months to years (Fabryka-Martin et al., 1993). Atmospheric sources dominate in waters older than 40 years and have concentration ratios of 500 ($^{36}\text{Cl}/\text{Cl} \times 10^{-15}$) in present-day waters but have been as high as 1500×10^{-15} over the past half million years. Anthropogenic sources dominate in young waters and reach values at Yucca Mountain as high as peak global fallout ($200,000 \times 10^{-15}$; Fabryka-Martin and Wolfsberg, presentation to NWTRB, 1996).

In rocks and minerals near the surface, ^{36}Cl is produced *in situ* by reaction of cosmic rays with ^{39}K , ^{40}Ca , and ^{35}Cl . This is termed spallation. The concentration of ^{36}Cl from this source is variable and depends on the age of exposure of rocks and minerals (with longer exposure times having higher ratios) as well as on their elemental composition. This source is thought to be of negligible importance at Yucca Mountain in comparison to the amount produced by atmospheric sources. Fabryka-Martin and others (1996) considered $^{36}\text{Cl}/\text{Cl}$ ratios in excess of 1500×10^{-15} to be indicative of bomb-pulse. It remains to be seen whether sufficient Cl can be mobilized from Cl at the surface to produce bomb-pulse ratios observed at depth. ^{36}Cl can also be produced *in situ* in deep subsurface rocks and ocean waters through neutron capture by ^{35}Cl . The estimated value at Yucca Mountain contributed by this source is 20-30 ($^{36}\text{Cl}/\text{Cl} \times 10^{-15}$) and is of little significance. The vast majority of Cl, including ^{36}Cl , is introduced to the earth's surface through precipitation.

The meteoric $^{36}\text{Cl}/\text{Cl}$ ratio is a result of two variable processes: cosmogenic production rate of ^{36}Cl in the atmosphere, and wet and dry deposition rates of stable Cl. Production of ^{36}Cl in the atmosphere is a function of atmospheric cosmic-ray intensity, which is inversely proportional to temporal variations in the earth's geomagnetic field intensity. Based on reconstructions of the paleomagnetic field intensity, ^{36}Cl production was perhaps double its present rate for much of the past 500 Ky (Fabryka-Martin et al., 1996). Variations in the stable Cl deposition rate are more difficult to reconstruct. These variations are a product of changing meteorologic patterns and changing source regions. The assumption is that the Cl deposition rate has varied $\pm 25\%$ relative to its present rate of $106 \text{ g Cl/m}^2/\text{yr}$ (Fabryka-Martin et al., 1993).

^{36}Cl is analyzed by collecting Cl leached from one to a few kilograms of broken rock, followed by filtering and precipitation as silver chloride (AgCl). After purification, the AgCl separate is analyzed by accelerator mass spectrometry (AMS). Analytical measurement and sample contamination are not usually sources of error. However, the rock is a possible source of contamination. Tuff contains Cl that can be released during reaming of the bit during drilling operations or during crushing in the laboratory. Rock Cl has lower $^{36}\text{Cl}/\text{Cl}$ ratios than background ratios, which would dilute the observed $^{36}\text{Cl}/\text{Cl}$ ratio. Since the $^{36}\text{Cl}/\text{Cl}$ ratio is inversely proportional to residence time or apparent age, this would indicate longer residence times. This explains why measured $^{36}\text{Cl}/$

Preliminary Conceptual Model of Flow Pathways based on ^{36}Cl and Other Environmental Isotopes

Cl ratios for borehole samples are systematically lower than values for ESF samples (Fabryka-Martin et al., 1993; Liu et al., 1995) because the method of sample collection in the ESF does not pulverize the rock.

^{36}Cl dating tends to indicate greater ages than ^{14}C methods by an order of magnitude (Liu et al., 1995). Uncorrected ^{14}C ages for pore water from the unsaturated zone and for perched water at Yucca Mountain have ranged from modern to 10 Ky (Yang, 1994; Yang et al., 1996) whereas uncorrected ^{36}Cl based ages have ranged from modern to 700 Ky (Fabryka-Martin et al., 1993). The apparent discrepancies may be attributed to one of the following reasons (Liu et al., 1995): 1) different transport mechanisms for carbon and chloride; 2) different magnitudes and timing of bomb-pulse signals; 3) mixing of waters from different flow paths with different apparent ages; and 4) inadequate methods for correcting for the effect of sample contamination by carbon or chloride from sources other than that in the infiltrating water. By adjustments using the Cl/Br ratio, measured $^{36}\text{Cl}/\text{Cl}$ ratios in rock samples are corrected for dilution of the meteoric component by rock Cl before calculating residence times from these data. However, the Cl/Br ratio itself is a source of uncertainty because the ratio varies in soils, alluvium, ground water and rock, and because of analytical difficulties in measuring extremely low Br concentrations.

10.1.2 Unsaturated Zone (UZ) Flow Model Calibration

Calibration of the unsaturated zone flow model relies on many different observations that are folded into conceptual models which balance the mass of gas, water, and energy. The conceptual models are then tested by numerical models which account for all of the observations. The preferred choice among alternate conceptual models is the one that most rigorously accounts for all of the data and observations. The calibration process involves testing each type of data or observation in the numerical model and then matching it to other observations. For example, the conceptual model of water flow must first account for the location and volume of perched water and then for perched water age (see ch. 7 of this volume; Wu et al.). Saturation and moisture tension from wells must be calibrated (see chapter 8 of this volume; Wu et al.). Next the concentration of environmental isotopes in wells and in the ESF must be accounted for (this chapter) along with fracture coating ages for their indication of flow pathways and residence times (see chapter 14 of this volume; Simmons et al.). ESF moisture balance must be considered to determine the degree of relative humidity and whether evaporation is occurring in fractures. Finally, data and observations from the Ghost Dance and other faults must be examined with respect to their influence on all of the above parameters. Similar types of calibration are done for the gas flow and heat transfer components of the unsaturated zone flow model.

Calibration of all of these components into one model is an ambitious undertaking. With the goal of producing a fully calibrated model which utilizes all available Yucca Mountain data for these parameters by June of 1997, we have accelerated efforts this year by incorporating as much information as possible.

Preliminary Conceptual Model of Flow Pathways based on ^{36}Cl and Other Environmental Isotopes

Although the results presented here are preliminary and will undoubtedly be refined as additional site characterization data become available, the calibration achieved for this 1996 model has given us a significant head start toward the final model.

10.1.3 Changes in the UZ Flow Model Based on Environmental Isotopes

The preferred conceptual flow model until recently at Yucca Mountain allowed for spatially variable flow and infiltration but was dominated by matrix flow (Montazer and Wilson, 1984). However, through site characterization data gathered since the mid-1980's from drill holes and from the Exploratory Studies Facility (ESF), it has become increasingly evident that flow along fast preferential pathways through fractures is a significant and perhaps the dominant flow regime in the unsaturated zone. Several lines of evidence point to the existence of fast flow pathways at Yucca Mountain. One of the most compelling lines is the existence and composition of perched water that is younger and different in composition from saturated zone water. Furthermore, in several locations perched water has been contaminated with polymer from drilling operations that reflects a recent infiltration pulse. A second important line of evidence is from environmental tracer tests such as ^{36}Cl and ^3H , and a third is derived from age dates of fracture-lining materials.

Wang and others (1993) investigated fast flow pathways at Rainier Mesa as a possible analog to wetter conditions at Yucca Mountain and encouraged the characterization of fast pathways through the Calico Hills unit based on their predictions. Yang (1992) identified fast pathways indicated by ^{14}C ages, ^3H , and major ion chemistry in UZ-16 and UZ-14 and in boreholes UZ-4 and UZ-5. Fabryka-Martin and others (1993) and Liu and others (1995) found evidence of bomb-pulse ^{36}Cl in boreholes UZ-14 and UZ-16 and in numerous neutron holes. In 1996 detailed studies in the area of the North Ramp of the ESF that included pneumatic and hydrologic property data as well as isotopic and geochemical data (Rousseau et al., 1996) provided supporting demonstration of the significance of fast pathways at Yucca Mountain. Their report was issued closely in time to reports on two other corroborating studies which synthesized geochemical and isotopic data: Yang and others (1996) interpreted chemical and isotopic data $\delta^3\text{H}$, ^{14}C , $\delta^{18}\text{O}$, and $\delta^{87}\text{Sr}$ from boreholes at Yucca Mountain, and Fabryka-Martin and others (1996) presented results of an extensive sampling, both systematic and feature-based, of evidence of ^{36}Cl with bomb-pulse signature at the repository horizon in the ESF in areas of through-going faults that served as preferential fast flow paths.

10.1.3.1 Perched Water

Perched water has been encountered at the base of the Topopah Spring Tuff, just above the contact between the lower nonlithophysal zone and the crystal-poor vitric zone, and in the top of the nonwelded to partially welded tuffs of the Calico Hills Formation in boreholes USW UZ-1, USW UZ-14, NRG-7a and SD-9 near the North Ramp. It was also found in UZ-16 and in SD-7 (see Figure 10.1.3.1.1). Major ion chemistry of this perched water is very similar to that of

Preliminary Conceptual Model of Flow Pathways based on ^{36}Cl and Other Environmental Isotopes

Calico Hills Formation pore water, a sodium-carbonate or sodium-bicarbonate type (Rousseau et al., 1996). The chloride concentration of the perched water, however (6×10^{-15} mg/l), is much lower than the chloride concentration of pore water obtained from the same interval (87.5 mg/l), indicating very little contribution of water from the matrix of the overlying rocks. Stable isotope data for $\delta^{18}\text{O}$ and deuterium (δD) are consistent with rapid, fracture infiltration with little or no evaporation. All samples represent the time period since last glaciation and are heavier in isotopic composition than saturated zone water (Benson and Klieforth, 1989). After correction of apparent ages for effects by dissolution of older caliche by infiltrating water, the age of perched water was estimated to be 4000-7000 years, an age that is much younger than any that could be derived using a matrix-to-matrix percolation model (Rousseau et al., 1996). In UZ-14 water ^{14}C values from the top 300 feet ranging from 70-95% modern carbon are similar to values for the Calico Hills Formation pore water, which are between 70-96% modern carbon at depths of 1400-1714 feet (Yang, 1992).

Figure 10.1.3.1.1

Cross-section of Yucca Mountain between Ghost Dance fault and Bow Ridge fault showing location of perched water at SD-7, location of bomb-pulse ^{36}Cl in neutron hole UZN-55 and location of bomb-pulse tritium in UZ-16

Even further evidence for rapid infiltration along fractures to depth is found in $\delta^{87}\text{Sr}$ signatures. The $\delta^{87}\text{Sr}$ signature of the perched water is +4.46%. This is similar to that for pedogenic calcite $\delta^{87}\text{Sr}$ of +4.4%) and calcite fracture fillings in the Yucca Mountain area, but dissimilar to that of the Topopah Spring Tuff [$\delta^{87}\text{Sr}$ of +1.5% to +9.6%; (Peterman and Stuckless, 1993)]. Saturated zone water has $\delta^{87}\text{Sr}$ values of +1.0 to +3.3%. These data indicate that perched water probably obtained its isotopic signature from dissolution of shallow surficial

Preliminary Conceptual Model of Flow Pathways based on ^{36}Cl and Other Environmental Isotopes

calcite during infiltration or during downward percolation through fractures (Marshall et al., 1993).

10.1.3.2 Locations of Indicators

Tritium concentrations were below detection limits (4 tritium units) at the same five locations in the ESF where bomb-pulse ^{36}Cl was found (Yang, presentation to NWTRB, 1996; see Figure 10.1.3.2.1). Greater than 30 tritium units (TU) is considered bomb-pulse. In Alcove 3 (where ^{36}Cl was not measured), tritium concentrations ranged from $6\text{--}12 \pm 4$ TU. In the Calico Hills Formation in UZ-16 concentrations of more than 100TU were detected (Yang et al., 1996). In Bow Ridge Fault gouge 40 m below ground surface and in UZ-N55 cuttings from a depth of 53 m, ^{99}Tc was detected. At these two locations, bomb-pulse ^{36}Cl was also detected (see Figure 10.1.3.1.1). In summary, bomb-pulse nuclides that behave in a chemically similar manner to ^{36}Cl , such as ^3H and ^{99}Tc (i.e., are not retarded in the flow system) are also detected at elevated levels some distance below the surface and confirm the existence of fast flow paths at least to those depths.

Figure 10.1.3.2.1

Map of UZ model showing model grid, trace of major faults, trace of ESF and boreholes where perched water was detected. Circles indicate locations where bomb-pulse concentrations of ^{36}Cl were found in the ESF.

Elevated tritium concentrations of pore water at several locations provide evidence for rapid, shallow fracture flow through the TCw and the PTn. Tritium profiles across these units indicated pore-water age inversions with older water overlying younger water. At one location age inversions were observed to a depth of 245 feet, just below the PTn-Topopah Spring contact (Rousseau et al., 1996). (Tritium concentration in UZ#4 ranges from 0-45 TU with a peak concentration at 150 feet; UZ#5 has a peak concentration of 75 TU at 105 feet; NRG-6 shows a peak of 30-150 TU broadly distributed from 175-245 feet) (Rousseau et al., 1996). Given the short half-life of tritium (12.5 years), the infiltration must have occurred within the last forty years or less.

**10.1.3.3
Corroborating Evidence of
Fast Paths**

Although bomb-pulse ^{36}Cl signatures at the repository horizon appear to be clear indicators of fast paths, greater confidence will be gained by evaluating lines of corroborating evidence, as well as examining contributions from other sources that could influence the signature and reconstruction of the past ^{36}Cl signal in the atmosphere. Other lines of evidence include: 1) surface calcite as an additional source of ^{36}Cl ; 2) examination of field relations and mineralogic textures, i.e. fluxes as estimated by fracture coatings and age dating of those coatings by U-series and ^{14}C methods [see chapter 14 of this volume; (Simmons et al.); 3) correlation of age dates with net infiltration estimates; and 4) measurement of other bomb-pulse nuclides such as ^3H , ^{137}Cs , ^{243}Pu , ^{99}Tc and ^{129}I .

Results of dating fracture coatings using ^{14}C and U-series dating are currently more in keeping with hypotheses of slow flux over long time periods (Paces, 1996) than with fast pathways. This supports hypotheses of several flow systems at Yucca Mountain, matrix flow, flow in fractures, flow in fractures/structural features, with some rapid and some very slow. The current distribution of U-series ages is quite broad, with a peak around 100-175 Ky and the youngest age at 37 Ky. Based on the concept of "continuous deposition", Paces (1996) estimated flux in "slow" fractures to be about 1×10^{-4} mm/yr. More extensive testing of models of calcite deposition and how they provide insights into flux estimates are needed.

**10.1.4
Objective of work**

The objective of this chapter is to apply knowledge from site characterization, e.g. chemical and isotopic composition of perched water, age of fracture filling materials, hydrologic properties of stratigraphic units, and geomorphology of drainage/infiltration areas to numerical models of fast flow through the repository horizon. The models are checked for consistency against results of other UZ model calibration parameters (e.g., see chapter 11 on percolation flux; Sonnenthal et al., and ch. 14 on fractures, which suggests the influence of north-south faults in focusing pathways; Simmons et al.) The numerical models are then used to predict which areas yet to be encountered in the ESF may provide additional evidence of fast flow paths and accordingly to devise an appropriate sampling and testing program that will allow not only better characterization of fast paths but also a greater understanding of flux at the repository horizon.

An understanding of flow pathways as indicated by environmental isotopes was already being incorporated into the unsaturated zone site-scale flow model when DOE requested that this aspect of the flow model receive greater emphasis because of concerns over the detection of bomb-pulse concentration of ^{36}Cl in the ESF. DOE requested that predictions be made as to where the Project can expect to find bomb-pulse concentrations in the remainder of the ESF that has not been excavated and in other areas of Yucca Mountain. Experience with field tracer tests at Raymond Quarry, the C-holes and in international programs (Grimsel laboratory, Stripa, etc.) has shown the difficulty of predicting where tracers will be found. Prediction of breakthrough has the greatest confidence in saturated sedimentary systems; in unsaturated rock the difficulty increases greatly and becomes even more difficult when the system is fractured, both of which are the case at Yucca Mountain. Compounding the challenge is the Project's very limited knowledge of the hydrologic characteristics of major faults and their role as flow pathways. However, without diversion of resources, we were able to combine insights gained from previous investigations of environmental isotopes (discussed above) with constraints of parameters of the UZ flow model, explained in other chapters of this report, to produce a preliminary flow model that incorporates environmental isotopes. Although the results presented here are preliminary and will be refined for the fully calibrated model in June 1997, the accelerated effort to incorporate environmental isotopes into the flow model has begun by testing conceptual models and comparing to improved our understanding of flow pathways in the unsaturated zone and will lead to a better focus for the FY97 model development.

Quality Assurance Pedigree of Data: The environmental isotope data in this chapter were taken from unqualified sources (non-Q) in published literature. Material properties were taken from chapter 3 of this report (Bandurraga et al.). See chapter 3 for detail of QA status. The Effective Continuum Model (ECM) module and radionuclide transport modules of TOUGH2 used in the numerical modeling of this chapter are presently being qualified in conjunction with this report (Wu et al., 1996). TOUGH2 Version 1.11 was qualified in February 1996 (Pruess et al., 1996).

10.2 Conceptual Model Development

The stratigraphy of Yucca Mountain is characterized by an alternating sequence of welded and non-welded ash flow and airfall tuff deposits (see Figure 10.1.1). The welded tuffs are characterized by low matrix porosities and permeabilities, but have high fracture densities. The non-welded tuffs have low fracture densities but relatively higher matrix porosities and permeabilities. All of the units were subject to varying degrees of alteration to clays and zeolites, which lowered their permeabilities in affected areas. Within the framework of this heterogeneous hydrogeologic system, three key factors affect flux at the proposed repository horizon: 1) variable patterns of near-surface infiltra-

tion, 2) spatial variability of flow through the Paintbrush Tuff non-welded unit (PTn), and 3) spatially variable material properties at the repository horizon.

Infiltration due to precipitation is variable, both spatially and temporally. Currently, estimates of net infiltration into the Tiva Canyon welded unit (TCw) vary spatially from 0 to 14 mm/yr (Flint et al., in review). Due to orthographic effects, more precipitation falls at higher elevations on Yucca Mountain, and to the north of the site. A greater fraction of precipitation falling on sideslopes and ridges, as opposed to alluvial channels and terraces, will become net infiltration (Flint, et al., 1994). Borehole studies have shown that infiltration processes are temporally variable, as well. Infiltration appears to move downward in episodic, transient pulses after rainfall events (Flint et al., 1994). These infiltration pulses can transit the extensively fractured TCw relatively quickly, as evidenced by apparent age inversions of water in the TCw and PTn.

Infiltration into the PTn is complex because fractures transmitting flux from the TCw generally terminate at the top of the PTn. Apparently few fractures cross all of the non-welded layers in the unit (Rousseau et al., 1996). Flow patterns within the PTn are affected by the microstructure and dipping of layers, small zones of alteration, and variability in permeability distribution in the unit. Existing fractures in the PTn make uncertain contributions to flux through the unit, as a result of permeability alterations arising from fracture coatings (see chapter 14, this volume). Because of its high porosity and high storativity, travel times through the matrix of the PTn are great. Flow penetrating the TCw may be diverted laterally either at the top or within the PTn, but the extent and volume of this flow is poorly understood, and as more information is obtained, lateral diversion appears to have less significance (Rousseau et al., 1996). The PTn unit is also transected by numerous faults that may act as both as conduits and barriers to subsurface fluid flow, depending on conditions.

The most important aspect of net infiltration is quantifying percolation flux at the potential repository horizon in the TSW unit. It is expected that the flux varies spatially and temporally in response to climatic changes and heterogeneity within the flow system. The ages of fracture- and lithophysal-cavity-filling materials within the TSW indicate that these materials were deposited by water percolating downward over hundreds of thousands of years. For the unfractured rock matrix of the TCw unit, TSW unit, and unaltered CHn unit, measured hydraulic conductivities are very small. Therefore, the rock matrix of these units would only be able to transmit water at an average velocity on the order of a fraction of a millimeter per year. Based on these properties and the net infiltration rates discussed above, flow through the rock matrix would require at least several thousand years to reach the potential repository horizon from the ground surface. Matrix saturation and water potential data from boreholes are consistent with these relatively low fluxes (<1mm/yr; Rousseau et al., 1996).

Current conceptual models for the hydrologic system at Yucca Mountain recognize that fractures and through-going faults may be conduits for episodic, rapid, gravity-driven, flow of water into and through the unsaturated zone. Montazer and Wilson (1984) stated that: "...nonuniform infiltration periodically produces moderately intense fluxes..." and "...pulses of infiltration may cause rapid percolation down through the Tiva Canyon welded unit and into the Paintbrush nonwelded unit." (Montazer and Wilson, 1984, p. 51). Evidence obtained from several studies at Yucca Mountain has established that water entering fractures in exposures of the highly fractured TCw unit at land surface following infrequent, intense storms is a major, if not the principal means, by which infiltration moves into the deep unsaturated zone. The largely unfractured and nonwelded PTn unit is considered likely to impede the downward flow of water that may be transmitted through the overlying TCw unit. Water entering the PTn unit is believed to be dispersed by imbibition into and diffusion through the rock matrix, and also may be diverted laterally along the eastward dipping beds of the unit. In this circumstance, the PTn unit may be a barrier to downward water flow that would restrict the movement of water into the underlying TSw unit. The absence of visible water inflow to the ESF from the enclosing rock mass and the results of apparent age determinations on fracture and cavity infilling materials in the TSw unit along the ESF main drift provide new evidence that the average downward water flux from the overlying PTn unit into and through the TSw unit is very low, as would be expected if the PTn is a flow barrier. Observations of localized occurrences of bomb-pulse ^{36}Cl in the ESF, however, imply that if the PTn is a barrier, it is not a uniformly continuous barrier to downward flow but is breached locally by pathways capable of rapid flow through the unit and into the underlying TSw unit.

For the present study, three conceptual models were examined that could account for rapid flow pathways through the PTn. Hypotheses examined included:

- A. Matrix: High saturations at the TCw/PTn contact create locally high hydraulic gradients, resulting in fast transport of ^{36}Cl through the matrix of the PTn. Once through the PTn, flow enters fractures in the TSw and migrates rapidly to depth (see Figure 10.3.1a);

Figure 10.3.1a

Hypothesis "A". This figure illustrates the conceptual model of fast pathway flow in which locally high saturations (shown in this figure as resulting from surface runoff) raise the unsaturated conductivity of the PTn unit to near its saturated value, resulting in fast transport of ^{36}Cl through the matrix of the PTn. Once through the PTn, flow enters fractures in the TSw and migrates rapidly to depth.

B. Fracture: Steady-state infiltration rates and rock properties are conducive to transport of bomb-pulse ^{36}Cl along continuous, high permeability fracture pathways (see Figure 10.3.1b);

Figure 10.3.1b

Hypothesis "B". This conceptual model of fast pathway flow proposes that ambient (steady state) infiltration finds conditions conducive to flow through high permeability fracture networks in the PTn.

- C. Fault: Transport of ^{36}Cl occurs as a result of rapidly transient pulses of infiltration along existing structural pathways (see Figure 10.3.1c).

Figure 10.3.1c

Hypothesis "C". This illustration presents the hypothesis that transport of ^{36}Cl occurs as a result of rapidly transient pulses of infiltration along existing structural pathways of high conductivity, such as faults, which transect the PTn at discreet locations.

A simple order of magnitude analysis was used to examine the reasonableness of hypothesis "A". If the average drained porosity is taken to be 0.15, the average vertical permeability of the PTn is probably on the order of $2\text{E-}13\text{m}^2$ (Ahlers, et al, 1996). Assuming a saturated thickness of 50 m for the PTn, a unit gradient, and evaluating the properties of water at 27°C , Darcy's law yields a travel time through the PTn of 40 days. Although this travel time is well within the range expected for fast pathway flow, this estimate is valid for *saturated* conditions. Deviation from saturation will cause a reduction in effective permeability, with a commensurate increase in travel times. For example, using the van Genuchten (1980) equation to relate saturation and relative permeability (with $m=0.163$, and a saturation of 0.5 for the PTn) yields a travel time of about 27,000 years. Clearly, for this conceptual model to remain valid, saturations must locally remain near 1.0 in the area of a fast pathway. Such high saturations of the PTn have not been observed to date in surface based boreholes or in the ESF. Furthermore, in order to maintain locally saturated conditions in the PTn, fluxes must be on the order of meters per year, and must persist for the duration of transit time (1 to 50 years). Since matrix saturation and water potential data from boreholes are consistent with low fluxes ($<1\text{mm/yr}$; Rousseau et al., 1996) and support the conclusions of long travel times through the matrix of the PTn, this model was dismissed.

In hypothesis "B" the PTn is continuously fractured for its entire thickness, and flow through the PTn is controlled by the permeability of the fracture(s) and the equilibrium established between the fractures and the matrix. This conceptual model was tested by Fabryka-Martin et al. (1996) for modeling fast pathway transport of ^{36}Cl . Many of the objections of hypothesis "A" are removed by hypothesis "B". Under saturated conditions (the lower bound on travel time) a fracture network with an effective permeability of 10^{-12} m^2 (effective hydraulic aperture = 0.004 mm) will conduct water through the PTn unit in a matter of minutes (subject to assumptions stated in the preceding paragraph). As in the analysis presented for hypothesis "A", travel times through the PTn under unsaturated conditions are much longer than for saturated conditions; however, even for very low saturations travel times through the PTn for the hypothetical 10^{-12} m^2 fracture remain within the 50-year time-frame for the transport of bomb-pulse ^{36}Cl . Our simulations qualitatively corroborated those conducted by Fabryka-Martin et al. (1996) which concluded that ^{36}Cl generated during above-ground nuclear testing could arrive at the proposed repository horizon in 50 years under hypothesis "B".

Hypothesis "B" offers a plausible theory for the transport of ^{36}Cl to the level of the ESF. Unfortunately, evaluation of the results of this conceptual model are not completely consistent with field evidence. The relatively low (as compared to a large, rapidly transient flux, as is proposed in hypothesis "C"), steady state fluxes assumed are more consistent with a "well-mixed flow" model of ^{36}Cl transport; however, modeling of tritium concentrations in UE25 UZ-16 by the United States Geologic Survey appears to support a piston-flow model of transport. Yang, et al., (1996) caution that no hydrologic system exhibits pure mixing- or piston-behavior, but nevertheless found their observations to be consistent with a piston-flow model.

In spite of this difficulty, hypothesis "B" cannot be entirely discounted. It remains a useful conceptual model for studying the effects of geologic and hydrologic parameters on the transport of ^{36}Cl , and for establishing bounds on flux and travel times. In order to investigate a conceptual model more consistent with the piston-flow model of transport, however, hypothesis "C" was chosen as the preferred conceptual model for this study.

Montazer and Wilson (1984) generally perceived transient fracture flow as ending at or in the PTn hydrogeologic unit, resulting in saturation build-up and lateral flow along the TCw/PTn contact. Early investigations of the effects of transient pulses on flux travel times at Yucca Mountain by Wang and Narasimhan (1986) found that small pulses were generally attenuated in the TCw, while larger pulses penetrated progressively deeper into the PTn. For the largest pulse case (12,500mm/yr for 0.2 years), the investigators found that the moisture front penetrated the upper part of the TSw unit in about 1,000 years after the application of the pulse. In this case the PTn unit was treated as a composite medium with no implicit fracturing (fracture and matrix properties of the

welded units were treated as a multiple interacting continuum). However, Buscheck and others (1991) and Nitao and others (1992) demonstrated through simulations that under certain conditions episodic fracture flow could transit the PTn with much shorter travel times. These investigators used a discrete fracture model and ponded conditions at the entrance to fractures of varying aperture (from 0.01 to 1.0 mm) to demonstrate the possibility of fast pathway flow at Yucca Mountain. The predicted travel times were strongly dependent on the assumed aperture of the fracture. For the assumed hydrologic properties, the 1.0 mm fracture was found to transmit infiltration to the level of the ESF in times on the order of 14 days, while flow through smaller fractures generally became matrix-dominated in the PTn. Other investigators working in the area of non-equilibrium fracture flow have obtained qualitatively similar results (see Zimmerman and Bodvarsson, 1995, 1996). Although the cited studies represent extreme conditions (i.e., ponded conditions at the fracture entrance), they provide modeling evidence that rapidly transient flow to the level of the ESF in less than 50 years is possible.

Field evidence also supports the feasibility of transient pulses reaching the level of the ESF. As mentioned in section 10.1, perched water encountered in USW UZ-14 was found to be contaminated with drilling polymers. In this case, a pulse of infiltration, generated by drilling operations at USW G-1, migrated several hundred meters laterally and vertically, within a few years. Although the infiltrating pulse was large (about 8,700,000 liters, Burger and Scofield, 1995), it demonstrates the possibility of transmitting episodic pulses through the unsaturated zone.

Due to the rapidly transient nature of the flow field inherent in hypothesis "C", analysis of this conceptual model is not amenable to simple analytical arguments such as were used for hypothesis "A". In addition, the difficulties in demonstrating the validity of one hypothesis over another are great. Rather than attempting a rigorous fast pathway model at a specific location at Yucca Mountain, we have chosen to use a very simple schematic model to examine the plausibility of hypothesis "C". This model is only the first step in incorporating environmental isotopes into a realistic model representative of actual site conditions. The details of these simulations are the subject of the following section.

10.3 Numerical Hypothesis Testing

10.3.1 Approach

The plausibility of the preferred conceptual model was tested numerically using the modular integrated-finite difference model TOUGH2 (Pruess, 1987, 1991). The grid for the schematic fast pathways model consisted of a two-dimensional mesh of 15 x 62 (930) blocks, thirty of which were boundary elements, fifteen representing the water table, and fifteen representing the land

Preliminary Conceptual Model of Flow Pathways based on ^{36}Cl and Other Environmental Isotopes

surface, not including the effects of alluvium or topography (see figure 10.3.1.1; both boundaries were considered to be at constant

Figure 10.3.1.1

Representation of grid for schematic fast pathways model. The fault zone is modeled as a rubbleized zone of high permeability occupying a single column of blocks (shaded area). All other blocks are combination matrix/fracture blocks represented by the equivalent continuum method (chapter 3, this volume). The bottom boundary is placed at the water table; the top boundary is at the land surface, exclusive of topography and alluvium (both boundaries are constant saturation, temperature, and pressure). The right-hand boundary is a no-flow boundary condition, while the left side of the grid is a symmetry boundary through the center of the fault zone (one-half of the fault zone is modeled explicitly). All dimensions are in meters. Drawing not to scale; some gridblocks are omitted for clarity.

Temperature, pressure, and saturation). Properties were assigned to the grid-blocks based on the most recent material property inversions from the unsaturated zone site-scale model (see chapter 3 of this volume) and were designed to be representative of the Yucca Mountain site. The properties assigned included both fracture and matrix properties (dual continuum) for the Tiva Canyon, Topapah Spring, and Calico Hills hydrogeologic units. Properties assigned to the Paintbrush non-welded units consisted of matrix properties only (single continuum), reflecting the predominantly unfractured character of the PTn as observed in the ESF. The cross-cutting fault was also modeled as single continuum. The grid was locally refined near the fault to allow accurate computation of saturations and capillary pressures in rapidly transient simulations.

Preliminary Conceptual Model of Flow Pathways based on ^{36}Cl and Other Environmental Isotopes

To represent a fast pathway as proposed in the preferred conceptual model, the hydrogeologic units were transected by a fault, whose properties were systematically varied. As mentioned in section 10.2, some information about fault permeabilities has recently become available as a result of pneumatic monitoring by the United States Geological Survey (Rousseau, et al., 1996), and analysis of pneumatic data by Lawrence Berkeley National Laboratory (Ahlers, et al., 1996); however, most fault properties have remained poorly constrained. In light of this uncertainty, the properties assigned to the fault blocks in the present model represent "generic" fault properties rather than those associated with a specific fault. The fault was intended to represent a narrow rubbleized zone of high permeability; effective single fracture apertures were calculated using the cubic law for ease of comparison. van Genuchten (1980) alpha parameters were approximated from capillary theory using the method of Wang and Narasimhan (1985) (see Figure 10.3.1.2), while porosities were calculated by dividing the effective fracture aperture by the gridblock width. Properties for the fault were assumed to be independent of depth, with the exception of horizontal permeabilities. Horizontal permeabilities in the fault were set equal to the fracture permeability of adjacent gridblocks, to stimulate mass flux out of the fault at a rate proportional to the bulk permeability of the surrounding geologic material.

Figure 10.3.1.2
Character curves for two simulated fault zones. Fault apertures shown are effective hydraulic apertures as calculated from the cubic law for comparison purposes.

10.3.2 Methods and Results

The primary modeling objective was to demonstrate the plausibility of the hypothesis that transport of ^{36}Cl through the PTn occurs as a result of rapidly

transient pulses of infiltration along existing structural pathways. Lateral spreading of ^{36}Cl below the PTn is discussed separately (see Chapter 14, Simmons, 1996). A secondary objective was to expand on investigations initiated by Fabryka-Martin, et al. (1996) as to what parameters might influence the transportation of ^{36}Cl to depth. To this end, simulations were conducted using two values of infiltration flux (0.1 mm/yr and 1.0 mm/yr) and two values of fracture permeability (effective hydraulic apertures of 0.5 mm and 1.0 mm), as well as several different sizes of transient infiltration pulses. These parameters and their associated values were chosen after a review of other modeling studies conducted in the area of fast pathway analysis; most notably those by Wang and Narasimhan (1986), Buscheck, et al. (1991), Nitao et al., 1992, and Fabryka-Martin et al. (1996). To evaluate the effect of different geologic conditions, PTn thicknesses of 20, 50 and 100 m were modeled. The 20 and 50 m thicknesses of PTn were chosen to approximately bracket measured thicknesses as reported by Moyer et al., (1995), while the 100 m thickness established an extreme case for comparison purposes.

A standard methodology was followed for each case modeled: a grid with appropriate material property assignments was run to steady state under the assumed ambient infiltration. After the model was equilibrated, an infiltration pulse was applied to the fault element blocks only for a period of one week (during this time, the non-fault blocks continued to receive infiltration at the ambient rate). The size of the pulses varied from a 2600 mm/yr to 26000 mm/yr (5 to 50 cm/wk), consistent in rate, but of shorter duration than pulses used by Wang and Narasimhan (1996), and smaller than those that would be expected from a ponded infiltration boundary condition (see section 10.4 for a discussion of the pulse sizes selected). This was followed by a recovery period of 50 years. A low concentration of a non-reactive tracer was added to all infiltration from the initiation of the pulse to the end of the recovery period, at which time the concentrations of tracer in the column were examined to determine the depth of penetration and spread of the infiltration pulse. The transport calculations were made using a radionuclide transport module written for the TOUGH2 code (Wu, et al., Chapter 4, this volume). The transport module is capable of simulating transport with dispersion (transverse and longitudinal), diffusion, decay, and adsorption; however, for the purposes of this study dispersion was neglected. Due to the short time of the simulations (50 years) as compared to the half-life of ^{36}Cl (50,000 years), radioactive decay was assumed to be negligible, as was retardation (^{36}Cl was assumed to act as a perfect tracer). The diffusion coefficient of ^{36}Cl in water was approximated as $1.0\text{E-}10\text{m}^2/\text{s}$. Although numerical dispersion is known to be a concern with transport modeling using finite difference schemes, it was felt that for an order of magnitude study, given the parameter uncertainties inherent in the geologic materials, this would be a second order effect that could be neglected.

Saturation and capillary pressure curves for the steady-state profiles responded appropriately to variations in infiltration rate and fault permeability.

Preliminary Conceptual Model of Flow Pathways based on ^{36}Cl and Other Environmental Isotopes

Greater fault permeability and lower infiltration rates dry the column slightly and cause a modest increase in capillary suction (capillary pressures become more negative), while lower fault permeability and higher infiltration rates have the opposite effect. The steady-state saturations and capillary pressure curves maintain an acceptable approximation of site conditions for all cases used in this study.

Figure 10.3.2.1 shows the effect of varying pulse size on tracer concentrations in the simulated fault. Concentrations represented in this plot (as in all plots, unless otherwise noted) are for a time 50 years after the beginning of pulse application. For the three cases shown, nominal infiltration rate, effective fault aperture, and PTn thickness were all held constant at 0.1 mm/yr, 1.0 mm, and 50 m, respectively.

Figure 10.3.2.1

Normalized concentrations of tracer as a function of depth below landsurface. The three pulses shown span one order of magnitude in size, ranging from 5.0cm/wk to 50cm/wk. The infiltration pulses were applied at the specified rate for one week, after which time the model was allowed to recover at ambient infiltration. The values of concentration shown are taken from a simulated high permeability pathway, fifty years after the initiation of the pulse.

As expected, concentration of arriving tracer at all depths is directly proportional to pulse size. For the two smaller pulses (5 cm/wk and 10 cm/wk), normalized concentrations at the level of the ESF are on the order of 1% (0.01 of input concentration). For the largest pulse, 50 cm/wk, concentrations at the ESF are greater than 60% of input concentration. Furthermore, it can be seen from the figure that, for the 50 cm/wk pulse, concentrations arriving at the water table are on the order of 10%, indicating travel times of less than 50 years to from the land surface to the saturated zone.

Preliminary Conceptual Model of Flow Pathways based on ^{36}Cl and Other Environmental Isotopes

The effects of different fault permeabilities (Figure 10.3.2.2) and infiltration rates (Figure 10.3.2.3) are also illustrated. For the cases illustrated in Figure 10.3.2.2, infiltration (0.1 mm/yr), PTn thickness (50 m), and pulse size (10 cm/wk) were all held constant. Effective fault aperture was varied by a factor of two, from 0.5 mm to 1.0 mm, a variation that spans the critical aperture size as noted in the studies of Buscheck et al., (1991) and Nitao et al., (1992). Similarly, pulse size (10 cm/wk), fault aperture (1.0 mm), and PTn thickness (50 m) were held constant for the cases shown in Figure 10.3.2.3, while the nominal infiltration rate was varied by an order of magnitude (0.1 mm/yr vs. 1.0 mm/yr).

Figure 10.3.2.2
Normalized concentrations of two different effective fault apertures: 0.5mm and 1.0mm.
Infiltration pulses shown are 10cm/wk.

Preliminary Conceptual Model of Flow Pathways based on ^{36}Cl and Other Environmental Isotopes

Figure 10.3.2.3

Normalized concentrations of tracer in a simulated fault zone as a function of depth below landsurface. Infiltration rates shown are 0.1mm/yr and 1.0mm/yr, for a pulse size of 10cm/wk.

In the cases presented in Figures 10.3.2.2 and 10.3.2.3, changes in concentrations of tracer arriving at the ESF in fifty years for the different cases were consistent with current thinking on fast pathways. An increase in the nominal infiltration rate resulted in a slightly more saturated column, decreasing capillary suction in the matrix and allowing more rapid travel times to the level of the ESF (figure 10.3.2.3). A similar trend is apparent in Figure 10.3.2.2; as fault permeability is increased, the arrival time of the tracer is decreased. The effect of different thicknesses of PTn on tracer concentrations, however, was unexpected. Figures 10.3.2.4 and 10.3.2.5 show variations in arrival concentrations of tracer as a function of pulse size and PTn thickness. For the cases shown infiltration and equivalent fault aperture are held constant at 0.1 mm/yr and 1.0 mm, respectively, while pulse size is varied from 5 cm/wk (figure 10.3.2.4) and 50 cm/wk (figure 10.3.2.5). For each figure, the thickness of the PTn was assigned values of 20, 50, and 100 m. As mentioned in section 10.2, the thickness of the PTn is believed to vary between approximately 20 and 50 meters; the 100 meter case was included to provide an extreme scenario for comparison purposes.

Preliminary Conceptual Model of Flow Pathways based on ^{36}Cl and Other Environmental Isotopes

Figure 10.3.2.4

Effect of PTn thickness on arrival concentrations of tracer at depth. Three thicknesses of PTn are shown: 20m, 50m, and 100m. Pulse size is 5.0cm/wk, effective fault aperture is 1.0mm. Thicknesses of 20 to 50m are generally representative of those found at the Yucca Mountain site; the 100m case is included as an extreme condition for comparison purposes.

Figure 10.3.2.5

Effect of PTn thickness on arrival concentrations of tracer as a function of depth, for a pulse size of 50cm/wk, and an effective fault aperture of 1.0mm.

10.4 Discussion of Results

To a varying degree, all factors tested in the numerical simulations affected the ability of infiltration pulses to penetrate to the depth of the ESF, particularly within the fifty year time-frame for bomb-pulse ^{36}Cl . System response to variation of parameters in each case was consistent with expectations based on prior experience and literature review. The sensitivity of the system to the parameters tested, however, was somewhat unexpected.

Previous investigators of fast pathways have generally assumed ponded boundary conditions at the fracture entrance (Buscheck, et al. 1991, Zimmerman, et al., 1996). Although this assumption is useful, the large fluxes associated with such a condition are probably not a reasonable approximation of field conditions. Results of the present study indicate that episodic fast pathway flow can occur with fluxes of a much smaller magnitude. Of those sensitivities evaluated in this study, the single most important factor in determining the concentration of tracer arriving at the horizon of the ESF is the volume of the infiltration pulse. In light of this sensitivity to pulse volume, an important question is whether the pulses used in these simulations are of a reasonable magnitude.

Although net infiltration is one of the most important parameters to be determined at Yucca Mountain, it is also one of the most difficult to measure. Estimates of net infiltration vary from slightly negative (net loss of moisture from the mountain) to about 10 mm/yr. Measurement of net infiltration is complicated by the heterogeneity of the Yucca Mountain site, among other factors. Recent estimates (Flint, et al., in review), show infiltration varying from zero to 14 mm/yr, depending locally on slope aspect, thickness of alluvial cover, extent of fracturing in the bedrock, and other factors (Figure 10.4.1). Unfortunately, a one-to-one correlation between temporally averaged estimates of infiltration and the size of rapidly transient pulses is not possible; however most, if not all, of the same considerations used by Flint, et al., (in review) to estimate net infiltration can be applied to pulse infiltration. In particular, the extent of fracturing at the tuff/alluvial contact and the thickness of overlying alluvium are important in determining the magnitude of infiltration pulse that could be generated by a storm event, or a series of storm events.

Preliminary Conceptual Model of Flow Pathways based on ^{36}Cl and Other Environmental Isotopes

Figure 10.4.1

Map of near-surface infiltration, showing the Exploratory Studies Facility. Locations of bomb-pulse levels of ^{36}Cl are marked as open circles. SOURCE: United States Geological Survey (Flint et al., in review).

Figure 10.4.2

Width of watershed basin needed to generate an infiltration pulse. By geometry, the basin width needed to generate an infiltration pulse is:

$$w_p = (D^2 \phi + V_p \tan \theta) / P \tan \phi$$

Preliminary Conceptual Model of Flow Pathways based on ^{36}Cl and Other Environmental Isotopes

where D is the thickness of alluvial cover at the center of the wash, P is the volume of precipitation per event, per area, ϕ is the porosity of the alluvium, and θ is the angle of inclination of the sides. The analysis neglects storage along the sidewalls and losses to evapotranspiration.

A simple geometric analysis can be used to illustrate the important factors in estimating infiltration (Figure 10.4.2). The width of basin (w_s) necessary to capture

sufficient precipitation from a single event (P = volume of precipitation/area) to saturate a thickness of alluvium lying in the bottom of the basin (thickness at the center of the basin = D) assuming a geometrically regular basin with sides inclined at some angle θ and porosity in the alluvium ϕ is:

$$w_s = D^2\phi/P\tan\theta \quad (10.1)$$

assuming no evapotranspiration or storage along the sidewalls. To transmit additionally a pulse of infiltration, volume V_p , through the alluvium requires a basin width $w_p > w_s$, where:

$$w_p = (D^2\phi + V_p \tan\theta)/P\tan\theta \quad (10.2)$$

Replacing the independent variables with values of $D = 0.5\text{m}$, $\phi = 0.40$, $\theta = 15^\circ$, $V_p = 0.5\text{m}^3/\text{m}$ (the maximum used in the simulations), and $P = 0.02\text{m}$ (2 cm/hr for one hour of precipitation, a reasonable value for a summer thunderstorm event) yields a basin width of 44 m. The major assumption of this analysis is that no storage of precipitation occurs along the sidewall. This is perhaps not overly conservative if the soil cover is thin, as it is on many ridges and side-slopes of the site (Flint et al., 1994), and the bedrock is fractured in conjunction with a fault zone. Some field evidence supports the supposition that zones of fracturing associated with faults at Yucca Mountain may be wide near the surface and taper with depth to a single feature or narrow zone near the PTn (W. Day, presentation to Nuclear Waste Technical Review Board, 1996). If this is the case, zones of fracturing associated with faults may by-pass soil cover and act to concentrate precipitation from large storm events and channel it to preferential pathways through the PTn.

Although the simple geometric analysis above indicates that pulses equivalent to those used in this study could, in theory, be generated at Yucca Mountain, the value of w_p will change for different independent parameters. In particular, w_p is especially sensitive to the depth of alluvium D , the only variable to which w_p has a functional dependence based on the square power. This is in agreement with the findings of other investigators, who have found that the deepest penetration of precipitation generally occurs where soils are thin

(ridges and sideslopes), while the shallowest infiltration is beneath thick alluvium in the bottoms of washes (Flint et al., 1994).

Patterns of ^{36}Cl deposition in near-surface boreholes also support a sensitive dependence between alluvial thickness and depth of penetration of an infiltration front. Unpublished results from ^{36}Cl analyses of cuttings from UZN-series boreholes (unsaturated zone boreholes for neutron moisture logging) indicate that areas of thick alluvial cover act to store infiltration, returning it to the atmosphere at a later time. For example, UZ-N54, which is located on an alluvial terrace with approximately 10 m of alluvium overlying bedrock, shows bomb-pulse concentrations of ^{36}Cl at depths of up to 3 m, while in UZ-N53, on a side-slope with about 15 cm of alluvial cover, bomb-pulse levels of ^{36}Cl can be found to depths greater than 60 m. Another borehole located in this same area, UZ-N55, where alluvial cover is on the order of 30 cm thick, demonstrates probable bomb-pulse ratios of ^{36}Cl to a depth of 80 m, at the top of the TSw unit. In the case of UZ-N55, transport through the PTn is believed to be associated with a fault zone, in agreement with the preferred conceptual model of this paper. Thus, field evidence as well as modeling results indicate that the most likely areas for development of fast pathways are in washes with thin alluvial cover which are transected by faults and prone to flooding.

Next to the size of the infiltration pulse, the numerical simulations show that fracture aperture is important in determining the depth of penetration of an infiltrating pulse of water. This is also in agreement with the results of other investigators. Buscheck et al. (1991) and Nitao et al. (1992), found the time for flow through a fracture to transit a unit (T) to be inversely proportional to the sixth power of fracture aperture ($T(b^{-6})$), assuming the validity of the cubic law (which the investigators note may not be applicable in all circumstances, but is illustrative).

While our study does show the PTn to have a role in attenuating infiltration pulses, the model is much less sensitive to PTn thickness than to the size of the infiltrating pulse or the effective fault aperture. Figures 10.3.2.4 and 10.3.2.5 illustrate this point. In these figures it can be seen that, for the two sizes of infiltration pulses shown in the graphs, tracer concentration arrivals at depth are only weakly dependent on the thickness of the PTn. The same is true for ambient infiltration flux rate. It was originally hypothesized that greater infiltration flux would result in higher matrix saturations, which would in turn weaken capillary suction in the matrix and lead to more rapid transmission of pulses and higher concentrations of tracer at depth. Although present (see figure 10.3.2.3), these effects are much less pronounced than expected. These results arise from the characteristic curves used for the fault properties. As discussed in section 10.3.1, fault characteristic properties were calculated from capillary theory, idealizing the rubbleized fault zone as a single fracture of equivalent effective hydraulic properties. One of the difficulties with this approach is the inability to make direct inferences from modeling results to field observations.

As has been discussed several times in this report, the characteristic curves and other properties (e.g., porosity) necessary for accurate modeling of flow in the fault zones at Yucca Mountain are presently unknown. The current study demonstrates only that the transport of ^{36}Cl as a result of transient pulse infiltration is *plausible*, given reasonable assumptions. Before accurate, site specific modeling of fast pathways can be undertaken these important properties must be better constrained.

10.5 Locations of Fast Pathways and Predictions

Our results indicate that in order for flow to occur along fast pathways, the following necessary conditions must be met:

- 1) A continuous, high-permeability pathway must exist to depth, and
- 2) A means of focusing infiltration and maintaining flux to the pathway must exist for a "sufficient" time.

The first condition implies an association between tectonic features and fast pathways. Faults cross-cut existing strata (as opposed to syngenetic fractures, which are generally strata-bound), and therefore represent features which could provide a "continuous, high-permeability pathway to depth". In fact, a strong correlation appears between elevated levels of ^{36}Cl and the presence of faulting. Of the five feature-based areas in the ESF which returned bomb-pulse ^{36}Cl ratios (some consisting of multiple samples), three are directly associated with mapped faults (four samples near the ESF station 2+00 were associated with the Bow Ridge fault, four samples between stations 18+90 to 19+50 were associated with the Drill Hole Wash fault, and six samples were near the Sundance fault, between stations 34+00 and 36+00), while the remaining two areas are close enough to known faults that a correlation is probable (a sample from station 12+44 is near the western edge of the Imbricate fault zone, and a sample from station 26+79 is close to the surface expression of an unnamed fault). Conversely, none of the systematic samples demonstrated bomb-pulse ^{36}Cl . The *existence* of a continuous-to-depth feature is not sufficient to provide a fast pathway, however. In addition to being continuous, the potential fast pathway must also have a *high permeability*. Historically, little data on the hydrologic properties of Yucca Mountain faults have been available, but recent analyses have provided some information on these critical parameters.

Utilizing data on barometrically-forced pressure fluctuations from instrumented boreholes at Yucca Mountain, Ahlers, et al. (1996) were able to infer properties for several faults in the vicinity of the ESF. By making reasonable assumptions, they calculated gas relative permeabilities in faulted sections of the TSw on the order of $1 - 20 \times 10^{-12} \text{ m}^2$, and through the PTn on the order of $0.2 \times 10^{-12} \text{ m}^2$. Although these values are somewhat small for non-equilibrium

fracture flow (a $20 \times 10^{-12} \text{ m}^2$ fracture would have an effective hydraulic aperture of 0.02 mm), they represent areal averages of permeability over hundreds or thousands of meters. In addition, because the permeabilities inferred are gas permeabilities, it is possible that locally high saturations in the faults could mask liquid permeabilities which are higher than those measured for gases. Given the heterogeneous nature of Yucca Mountain, the existence of areas of permeability sufficient to sustain episodic fracture flow within faults is a reasonable assumption.

The second necessary condition may be satisfied in channels of washes that transect the site. As discussed in section 10.4, Flint et al. (1994) found that the depth of penetration of an infiltration front was inversely proportional to the thickness of the alluvial cover. They found that: "...when surface flow is negligible, the deepest infiltration was found in the ridgetops, and the shallowest infiltration was observed in the washes...". Following significant runoff events, however, they noted: "...large volumes of water often infiltrated more than 5 meters into the soil in the washes..." (Flint et al., 1994). These observations suggest that the most likely point of origin for infiltration pulses is the bottoms of washes that are subject to flash flooding and have alluvial cover thickness of (much) less than 5 m. As discussed in the preceding section, the basin size necessary to generate a pulse of infiltration is directly proportional to the square of the thickness of alluvial cover (among other factors). Thick alluvium tends to store potential infiltration and return it to the atmosphere by evapotranspiration. An absence of alluvium would seem to be ideal for generating an infiltration pulse; however, without the ability to store some water at the surface, the duration of the event may be too short to generate the necessary pulse of infiltration. A thin alluvial cover will moderate the infiltration pulse, but also act to sustain flux into the high-permeability pathway. The presence of fault splays, which may act to concentrate runoff and funnel it to a through-going structural feature, will also increase the likelihood of fast pathway formation.

From this discussion we can select candidate areas for fast pathways. A candidate area will be in an active wash with thin alluvial cover, preferably with a large basin area to collect runoff. In addition, the candidate area will be in close proximity to a high permeability fault zone. With the exception of bomb-pulse ^{36}Cl associated with the Bow Ridge fault (four samples near ESF station 2+00), all known detections of bomb-pulse ^{36}Cl are located near active washes (see Figure 10.5.1). Bomb-pulse ^{36}Cl detections associated with the Bow Ridge fault are not believed to be representative because their occurrence in the ESF is above the PTn hydrostratigraphic unit. The Drillhole Wash fault ^{36}Cl detections (ESF stations 18+90 to 19+50) are located proximal to thicker areas of alluvium (4-5m); however, this wash is known to flood, and is so marked on the "Flood Potential of Fortymile Wash" map (U.S. DOE, 1995). This increases the probability that at times in the recent past sufficient moisture was available to saturate the alluvium and generate an infiltration pulse in spite of the relatively thick alluvial cover in this wash. The other ^{36}Cl detections (ESF stations 12+44,

Preliminary Conceptual Model of Flow Pathways based on ^{36}Cl and Other Environmental Isotopes

26+79, and 34+00 to 36+00, as well as recent detections at stations 43+63 and 44+20) are all located in areas of thin alluvial cover, beneath the upper regions of washes whose lower regions are known to be flood prone (U.S. DOE, 1995). The association of the known bomb-pulse ^{36}Cl occurrences with faults has already been discussed.

Figure 10.5.1

Map of alluvial thickness at the Yucca Mountain site, showing the Exploratory Studies Facility and major faults. Open red circles denote locations of known bomb-pulse ^{36}Cl samples; filled red circles show approximate locations of candidate areas for bomb-pulse ^{36}Cl .

Based on these considerations, we chose four candidate areas that will be intersected by the ESF as likely zones for the detection of bomb-pulse levels of ^{36}Cl . These areas are noted on Figure 10.5.2, and are located near ESF stations 50+00, 55+00, 57+00 to 61+00, and station 68+00. The first three of these locations are beneath upper regions of washes whose lower regions are prone to flooding (U.S. DOE, 1995), in areas of thin alluvial cover (Flint et al, in review), and proximal to the surface trace of the Ghost Dance fault (Day, et al., in review). The fourth is beneath a similarly flood-prone wash, in close proximity to the Dune Wash fault (Day, et al., in review).

These "predictions" should be viewed with some caution. In particular, the numerical simulations indicate the most important properties with respect to fast pathways are those of the fault or fracture zone. Although the candidate sites were chosen by determining areas most conducive to fast pathway formation, properties of the fault zones in these candidate areas are not well constrained. Pneumatic data from UZ-7a indicates that the Ghost Dance fault is a high permeability pathway in the area of ESF station 50+00 (see chapter 6 of this volume); however, as mentioned earlier, fault permeabilities determined from pneumatic data represent averages over relatively large spatial scales. There is, therefore, no guarantee that a high permeability pathway will intersect the alignment of the ESF in the area of the candidate sites. In addition, we expect lateral spreading of flux along the trace of the fault (as appears to be the case along the main test level of the ESF) to be more significant than spreading perpendicular to the fault. Testing along the south ramp of the ESF, therefore, may be less likely to encounter bomb-pulse isotopes than testing along the main test level. These factors are effects of the innate heterogeneity of Yucca Mountain, which makes any predictions of fast pathway locations extremely difficult. It is worth mentioning that, even in the saturated zone, the prediction of tracer tests in fractured, heterogeneous geologic media is very difficult. These difficulties are amplified by orders of magnitude in the unsaturated zone. Nevertheless, in our view, the candidate sites described above offer the highest probability for the detection of fast pathways, and should be considered for detailed sampling for ^{36}Cl as well as other environmental tracers.

10.6 Summary and Conclusions/Recommendations

Summary

1. Fast flow pathways exist at Yucca Mountain as indicated by the pressure of Lamb-pulse tritium, ^{36}Cl and young perched water.
2. We expect the PTn to constitute a major barrier to infiltration into the TSw, except in areas where it is breached by major through-going faults. Our preferred conceptual model, based on evaluation of these alternatives, is one in which transport of ^{36}Cl occurs as a result of rapidly transient infiltration pulses along existing structural pathways.
3. In order for flow to occur along fast pathways, a continuous, high-permeability pathway must exist to depth and a means of focusing infiltration to the pathway must exist.
4. Formation of a fast pathway is very sensitive to the characteristics of the pathway, i.e. fault-zone permeability, pulse volume, depth of alluvial cover, and characteristic curves.

Preliminary Conceptual Model of Flow Pathways based on ^{36}Cl and Other Environmental Isotopes

5. Four areas that will be intersected by the ESF are candidate sites for detection of bomb-pulse concentrations of ^{36}Cl . These are located near ESF stations 50+00, 55+00, 57+00 to 61+00, and station 68+00. All four are beneath upper regions of washes whose lower regions are prone to flooding, all are in areas of thin alluvial cover, and all are close to surface traces of faults.
6. Penetration of recent water into the TSw unit is indicated by bomb-pulse ^{36}Cl in fractures of the ESF. However, bomb-pulse signals by themselves are not indicative of the amount or distribution of ground water flux within the unsaturated zone. Further testing and modeling is necessary to discriminate between fast pathways along major, through-going structures such as faults, and randomly located features such as interconnected fracture networks.
7. Fast pathways alone are not detrimental to repository performance unless it can be shown that fluxes along those pathways are significant. Cumulative results of all of the ^{36}Cl sampling suggest that the fraction of bomb-pulse water at the repository horizon may be a very small fraction of total flow at this depth. Most of the ^{36}Cl was not deposited by rapid flow. Therefore, the ^{36}Cl data agree with existing conceptual models of the Yucca Mountain ground water flow system in that a small volume of ground water representing a small fraction of the total flow can travel rapidly through the unsaturated zone, especially in the vicinity of structural features that penetrate the TSw. The difference between occurrence of ^{36}Cl at the repository horizon and the significance of ^{36}Cl occurrence is a regulatory issue.

These statements are based on non-Q data but are scientifically valid.

Recommendations

1. Because of the sensitivity of fast pathway flow to fault characteristics, an increased emphasis on characterization of fault properties at the surface and in the ESF should be a high priority for the Project. Particular emphasis should be placed along the main test level with attention paid to lateral spreading along north-south trending fractures. This will allow the necessary refinement of the site-scale flow model to include variation of fault properties with depth.
2. A sampling program in the ESF should include areas near structural features, particularly those below areas that meet other criteria at the ground surface, based on predictions of location of fast pathways near faults, as described in section 10.5
3. Determination of flux should receive high priority for investigation through *in situ* field tests and confidence-building through modeling, because flux is the most important parameter needed by PA.

4. Many lines of investigation should be pursued to further understand the significance of fast pathways to repository performance. Preliminary results regarding the bomb-pulse ^{36}Cl concentrations observed at repository depth in the TSw may be significant to the predicted long-term performance of the potential Yucca Mountain repository, but the observations should be combined with all other direct and indirect indicators of percolation flux and its distribution in space and time between fractures and matrix to provide confident estimates of these important performance parameters. ^{36}Cl observations should be one part of the investigations and continued sampling (in the ESF especially below areas of thin alluvial cover and near structural features), analysis, interpretation, and modeling to explain the ^{36}Cl distribution should be undertaken with the aim of defining the correlation, or lack thereof of, such observations with mappable structural features. If these features are randomly located and therefore cannot be detected or avoided, then determining the flux distribution in the features with confidence and the continuity of the features with depth will be important determinants in predicted overall performance of the repository over long time periods.

10.7 References

- Ahlers, C.F., T.M. Bandurraga, G.S. Bodvarsson, G.Chen, S. Finsterle, and Y.S. Wu, Summary of model calibration and sensitivity studies using the LBNL/USGS three-dimensional unsaturated zone site-scale model, Yucca Mountain Project Milestone 3GLM107M, Lawrence Berkeley Laboratory, Berkeley, CA, 1995.
ACCN: MOL.19960208.0091-0097
DTN: LB092995312293.001 (Non-Q)
- Ahlers, C.F., C. Shan. C. Haukwa, A.J.B. Cohen, and G.S. Bodvarsson, Calibration and prediction of pneumatic response at Yucca Mountain, Nevada using the LBNL/USGS three-dimensional site-scale model of the unsaturated zone, Yucca Mountain Project Milestone OB12M, Lawrence Berkeley Laboratory, Berkeley, CA, 1996.
- Benson, L.V., and H. Klieforth, Stable isotopes in precipitation and ground water in the Yucca Mountain region, South Nevada: paleoclimatic implication: Geophysical Monograph 55, pp. 41-59, 1989.
- Burger, P.A., and K.M. Scofield, Perched water at Yucca Mountain -- implications on the Exploratory Studies Facility, Nye County, Nevada, 26 pp., 1996.
- Buscheck, T.A., J.J. Nitao, and D.A. Chesnut, The impact of episodic nonequilibrium fracture-matrix flow on geological repository performance, American Nuclear Society FOCUS '91 Conference on Nuclear Waste Packaging, Las Vegas, NV, September 29-October 2, 1991, 1991.

Preliminary Conceptual Model of Flow Pathways based on ^{36}Cl and Other Environmental Isotopes

- Day, W.C., C.J. Potter, D.S. Sweetkind, and R.P. Dickerson, Bedrock geologic map of the central block area, Yucca Mountain, Nevada, U.S. Geological Survey Preliminary Map (not for distribution), mapping through 4/26/96 (in review).
- Day, W.C., and S. Beason, Geologic structure at Yucca Mountain, presentation to U.S. Nuclear Waste Technical Review Board, Denver, CO, July 9-10, 1996.
- Fabryka-Martin, J.T. and A.V. Wolfsberg, Hydrologic flow paths and rates inferred from the distribution of chlorine-36 in the ESF, presentation to Nuclear Waste Technical Review Board, Denver, Colorado, July 9-10, 1996.
- Fabryka-Martin, J. T., P.R. Dixon, S. Levy, B. Liu, H.J. Turin, and A.V. Wolfsberg, Systematic sampling for chlorine-36 in the Exploratory Studies Facility, LA-CST-TIP-96-001, Milestone 3783AD, Los Alamos National Laboratory, Los Alamos, NM, 61 pp., 1996.
- Fabryka-Martin, J.T., S.J. Wightman, W.J. Murphy, M.P. Wickham, M.W. Caffee, G.J. Nimz, J.R. Southon, and P. Sharma, Distribution of chlorine-36 in the unsaturated zone at Yucca Mountain: an indicator of fast transport paths, Proceedings of FOCUS '93: Site Characterization and Model Validation, (American Nuclear Society, La Grange Park, Illinois) Las Vegas, Nevada, September 26-29, 1993, pp. 58-68, 1993.
- Flint, L.E., A.L. Flint, and J.A. Hevesi, Shallow infiltration processes in arid watersheds at Yucca Mountain, Nevada, in Proceedings of the Fifth International High Level Radioactive Waste Management Conference, (American Nuclear Society, La Grange Park, Illinois), Las Vegas, Nevada, May 22-26, 1994, pp. 2315-2322, 1994.
- Flint, A.L., J.A. Hevesi, and L.E. Flint, Conceptual and numerical model of infiltration for the Yucca Mountain area, Nevada, U.S. Geological Survey Water Resources Investigation Report 96-xxxx (in review).
- Liu, B., J.T. Fabryka-Martin, A.V. Wolfsberg, B. Robinson, and P. Sharma, Significance of apparent age discrepancies in water ages derived from atmospheric radionuclides at Yucca Mountain, Nevada, in Water Resources at Risk, W.R. Hotchkiss, J.S. Downey, E.D. Gutentag, and J.E. Moore, eds., (American Institute of Hydrology, Minneapolis, Minnesota), pp. NH-52-NH-62, 1995.
- Marshall, B.D., J.F. Whelan, Z.E. Peterman, K. Futa, S.A. Mahon, and J.S. Stuckless, Isotopic studies of fracture coatings at Yucca Mountain, Nevada, USA, in Water-Rock Interaction, Proceedings of the Seventh International Symposium on Water-Rock Interaction (WRI-7), Park City, Utah, July 13-18, 1992, A.A. Balkema, Rotterdam and Brookfield, Capetown, South Africa, pp. 737-740, 1992.
- ACCN: NNA.19921029.0034
DTN: GS920208315215.004

Preliminary Conceptual Model of Flow Pathways based on ^{36}Cl and Other Environmental Isotopes

- Montazer, P., and W.E. Wilson, Conceptual hydrologic model of flow in the unsaturated zone, Yucca Mountain, Nevada: U.S. Geological Survey Water Resources Investigation Report 84-4345, 55 p., 1984.
- Moyer, T.C., J.K. Geslin, and L.E. Flint, Stratigraphic relations and hydrologic properties of the Paintbrush Tuff (PTN) nonwelded hydrogeologic unit, Yucca Mountain, Nevada, U.S. Geological Survey Open-File Report 95-397, 164 pp., 1995.
- Nitao, J.J., T.A. Buscheck, and D.A. Chesnut, The implications of episodic non-equilibrium fracture-matrix flow on site suitability and total system performance, in Proceedings of the Third International High-Level Radioactive Waste Management Conference, (American Nuclear Society, La Grange Park, Illinois), Las Vegas, Nevada, April 12-16, 1992, pp. 279-296, 1992.
- Paces, J. B., Memorandum to R.W. Craig dated February 23, 1996, concerning "Submission of Milestone 3GQH455", 1996.
DTN: GS960208315215.001 Q
- Peterman, S.E. and J.S. Stuckless, Isotopic evidence of complex ground-water flow at Yucca Mountain, Nevada, in Proceedings of the Fourth International High-Level Radioactive Waste Management Conference, Las Vegas, Nevada, April 26-30, 1993, (American Nuclear Society, La Grange Park, Illinois), p. 1559-1566, 1993.
- Pruess, K., TOUGH User's guide, Report LBL-20700, Lawrence Berkeley Laboratory, Berkeley, California and Nuclear Regulatory Commission Report NUREG/CR4645, Washington, DC., 78 pp., 1987.
- Pruess, K., TOUGH2, a general-purpose numerical simulator for multiphase fluid and heat flow, Report LBL-29400, Lawrence Berkeley Laboratory, Berkeley, California, 102 pp., 1991.
- Pruess, K., A. Simmons, Y.S. Wu, and G. Moridis, TOUGH2 software qualification, Report LBL-38383, Lawrence Berkeley National Laboratory, Berkeley, California, 131 pp., 1996.
- Rousseau, J.E., E.M. Kwicklis, and D.C. Gillies, eds., Hydrogeology of the unsaturated zone, North Ramp area of the Exploratory Studies Facility, Yucca Mountain, Nevada, U.S. Geological Survey Water Resources Investigations Report 96-xxx, 267 pp., 1996.
- U.S. Department of Energy, Yucca Mountain Site Characterization Project Site Atlas 1995, volume 1, prepared by EG&G Energy Measurements, 1995.
- van Genuchten, M. Th., A closed-form equation for predicting the hydraulic conductivity of unsaturated soils: Soil Science Society of America Journal, 44, p. 892-898, 1980.

Preliminary Conceptual Model of Flow Pathways based on ^{36}Cl and Other Environmental Isotopes

- Wang, J.S.Y., N.G.W. Cook, H.A. Wollenberg, C.L. Carnahan, I. Javandel, and C.F. Tsang, Geohydrologic models of Rainier Mesa and their implications to Yucca Mountain in Proceedings of Fourth International High-Level Radioactive Waste Management Conference, (American Nuclear Society, La Grange Park, Illinois), Las Vegas, Nevada, April 26-30, 1993, pp. 675-682, 1993.
- Wang, J.S.Y. and T.N. Narasimhan, Hydrologic mechanisms governing partially saturated fluid flow in fractured welded units and porous non-welded units at Yucca Mountain, Report SAND-7114, Sandia National Laboratories, Albuquerque, New Mexico, 73 pp., 1986.
- Wilson, M.L., J.H. Gauthier, R.W. Barnard, G.E. Barr, H.A. Dockery, E. Dunn, R.R. Eaton, D.C. Guerin, N. Lu, M.J. Martinez, R. Nilson, C.A. Rautman, T.H. Robey, B. Ross, E.E. Ryder, A. R. Schenker, S.A. Shannon, L.H. Skinner, W.G. Halsey, J. Gansemer, L.C. Lewis, A. D. Lamont, I.R. Triay, A. Meijer, and D.E. Morris, Total system performance assessment for Yucca Mountain - SNL Second Iteration (TSPA-1993), Sandia National Laboratories Report SAND93-2675, Sandia National Laboratories, Albuquerque, NM, 1994.
ACCN: NNA.19940112.0123
- Wilson, M.L., TSPA insights into impacts of climate and chlorine-36, presentation to U.S. Nuclear Waste Technical Review Board, Denver, Colorado, July 9-10, 1996.
- Wu, Y.S., S. Finsterle, P. Fraser, C.F. Ahlers, and A. Simmons, Software qualification for ITOUGH2 and various equation-of-state (EOS) modules and auxiliary modules for TOUGH2 and ITOUGH2, Report LBL-xxxx, Lawrence Berkeley National Laboratory, Berkeley, CA, (draft).
- Yang, I.C., Flow and transport through unsaturated rock - data from two test holes, Yucca Mountain, Nevada, in Proceedings of Third International High-Level Radioactive Waste Management Conference, (American Nuclear Society, La Grange Park, Illinois), Las Vegas, Nevada, April 12-16, 1992, pp. 732-737, 1992.
ACCN: NNA.19930112.0137
DTN: GS920908312272.011 (Non-Q)
- Yang, I.C., G.W. Rattray, and P. Yu, Interpretations of chemical and isotopic data from boreholes in the unsaturated zone at Yucca Mountain, Nevada, U.S. Geological Survey Water Resources Investigations Report 96-4058, 58+ pp., 1996.
- Zimmerman, R.W. and G.S. Bodvarsson, Coupling of the semi-analytical dual-porosity simulation procedure to the LBNL/USGS site-scale model of the unsaturated zone at Yucca Mountain, Yucca Mountain Project Milestone 3GLS101MM, 1996.

SUBMODEL OF PERCOLATION FLUX AT THE REPOSITORY

E. Sonnenthal, S. Finsterle, and G.S. Bodvarsson

August 1996

11.1 Introduction

Quantification of the percolation flux at different spatial scales is necessary for assessing possible interactions of meteoric water with the proposed repository at Yucca Mountain. The large-scale global flux predicted by coarsely gridded site-scale models will help determine the maximum potential for waste dissolution and transport to the saturated zone. For determination of smaller more localized fast paths and channels that form because of smaller scale heterogeneities, one must employ submodels. It is to be expected that "fast" flow will occur at all scales and the important task of quantifying these flow rates is a challenge.

The current three-dimensional UZ site-scale model has a spatial discretization on the order of 100m horizontally and 10 to 50m vertically. It is hoped that this spatial discretization is sufficient to resolve lateral and vertical fluxes to the extent warranted by the existing data set and that required by the performance assessment abstraction team. It is important to quantify to some extent the accuracy of the UZ model, both in terms of grid discretization errors and also in terms of heterogeneities at various scales. In this chapter we develop a submodel of the three-dimensional UZ model that is used to investigate grid effects and the effects of heterogeneous fracture and matrix properties.

The UZ submodel considered covers an area of 160m E-W by 100m N-S and extends from the ground surface to the water table. The grid element dimensions of the horizontal grid is 10m with a variable vertical spacing, but generally of the same order. All geological complexities, such as layering and dips, are retained from the larger scale UZ model. Thus, this model provides a much-needed link between the geologically realistic UZ model and the more abstracted smaller scale drift-scale models, such as those developed by Birkholzer and coworkers at LBNL (Birkholzer et al., 1996). It is expected that the submodel developed in this chapter will provide the boundary conditions for future work on the drift-scale models in FY97.

The 10m resolution of the submodel grid will allow us to examine the possible spatial variations in percolation fluxes at a scale an order of magnitude smaller than is possible with the current UZ model. Although we are considering only the steady-state fluid fluxes in this work it will be also be important in future studies to quantify the effects of short periods of increased precipitation resulting in transient infiltration pulses above the repository horizon.

11.2 Approach

Criteria for the selection of the submodel are based on geologic, modeling and verification considerations. Evaluation of the flow patterns, fluid fluxes, and saturations generated by three-dimensional UZ model simulations (see chapter 8; Wu et al., 1996), help in selection of the submodel site and allow for direct comparison with the submodel simulation results. Development of the submodel entails the creation of a three-dimensional grid and the assignment of hydrogeologic unit thicknesses, geometries, and rock properties. The fracture and matrix permeabilities, relative permeabilities, porosities, thermal properties, and boundary conditions must be consistent with the UZ model. We then model the steady-state fluid fluxes, temperatures, and liquid saturations using the TOUGH2 code (Pruess, 1987; 1991). To model the effect of permeability heterogeneities on the steady-state fluid fluxes, a stochastic permeability field generated by simulated annealing is used to modify the UZ model permeabilities within the submodel.

11.3 Quality Assurance Status of Data and Software Used In This Chapter

No quality-affecting work was performed in this study. Quality-affecting data was not developed in this work. The rock properties and geologic data used in the model simulations are non-Quality Assurance (Q) data. The simulation code TOUGH2 is Q. The simulating annealing code SIMAND3D is non-Q. The ITOUGH2 code is Q.

11.4 Selection of a Submodel of the UZ Model

It is important that the geologic characteristics of the submodel are representative of the repository area. The data sources from which the implemented geology and rock properties are derived (i.e., boreholes, the Exploratory Studies Facility (ESF), and drifts off the ESF; the North and South Ghost Dance Fault alcoves and the thermal alcove) should be close to the submodel area. From a modeling perspective, the local flow field near the repository horizon in the area surrounding the submodel should be predominantly vertical. This simplifies the assignment of boundary conditions imposed at the sides of the submodel, because it is then unnecessary to prescribe local horizontal fluxes.

A submodel was defined from the UZ model (Fig 11.4.1) that is bounded on the east by the Exploratory Studies Facility (ESF) and on the west by the trace of the Ghost Dance Fault (GDF). The submodel is bounded to the north by the North Ghost Dance Fault Alcove. The dimensions of this inner rectangular submodel are 160 m (E-W) by 100m (N-S) and from the top of the Tiva Canyon unit

(TCw) to the Prow Pass formation at the level of the water table model layer (PP3vp to PP2zp). In addition to the site's proximity to the ESF, the alcove, and the GDF, the trace of the roughly NW-trending Sundance Fault passes diagonally across the submodel domain. In further studies, the inclusion of fault properties from the Sundance Fault will allow for the evaluation of potential "fast paths", as indicated by the presence of bomb pulse ^{36}Cl (Faybeyha-martin et al., 1996) at the level of the repository. The area adjacent to the North GDF Alcove is the proposed site for the Percolation Flux Test, an array of horizontal boreholes spaced approximately 10m apart from which data will be obtained on liquid saturations, temperatures, and fluxes. There will be pneumatic data, permeabilities, temperatures, and fracture geometries and sizes from the ESF and the alcove itself, which will be compared to the submodel results.

Location of Submodel and Potential Percolation Study Area

Figure 11.4.1

Map view of submodel. The Ghost Dance Fault and the projected positions of the ESF and North Ghost Dance Fault alcove are boundaries to the submodel.

11.5 Geology of the Submodel Area

An E-W cross-section of Yucca Mountain, taken in the vicinity of the submodel area, shows the hydrogeological units and offsets of the major faults (Fig. 11.5.1). The submodel area is located to the west of the Ghost Dance Fault,

Figure 11.5.1

E-W cross-section of Yucca Mountain showing hydrogeological units and major faults. Details can be found in chapter 2 (Bandurraga et al., 1996).

which has a vertical offset of approximately 23 to 29 meters locally (see chapter 2: Bandurraga et al., 1996).

Given the small area of the submodel, the geological data obtained from the UZ model would be expected to be fairly uniform over the extent of the submodel. Although the stratigraphic relations are uniform over the submodel area, substantial variations exist in the unit thicknesses (Table 1). One notable rock property boundary is adjacent to the submodel in the region of coarse grid elements surrounding it, dividing a much less permeable zeolitized region of the CHn geologic unit (CH1zc) to the east from a vitric region (CH1vc) to the west. The trace of the NW-trending Sundance Fault zone crosses diagonally across the center of the submodel and is a normal fault, having displacements of zero to 35 feet along its 1500 ft. length (Rousseau et al., 1996). A detailed discussion of the geology, stratigraphy and hydrogeological units is presented in Chapter 2 (Bandurraga, 1996).

For reference, a range of thicknesses and vertical matrix and fracture permeabilities for the hydrogeological units present in the submodel are given in Table 11.5.1. All rock transport property (fracture and matrix permeabilities), porosities, van Genuchten parameters for fractures and matrix, and residual saturations were determined by inverse modeling of borehole data and are described in detail in Chapter 3 (Bandurraga et al., 1996).

Table 11.5.1. Typical Thicknesses and Permeabilities of Hydrogeological Units in Submodel			
Unit	Thick- ness (m)	Vertical Permeability (m ²)	
		Matrix	Fracture
TCw11	25 - 55	1.55e-18	5.23e-12
TCw12	6	1.14e-16	6.40e-12
TCw13	3	6.41e-17	5.76e-12
PTn21	3	2.40e-13	-
PTn23	3	2.30e-15	-
PTn24	5 - 6	3.26e-15	-
PTn25	10 - 16	4.41e-13	-
TSw31	3 - 4	1.62e-16	6.31e-12
TSw32	35 - 45	6.14e-15	4.22e-12
TSw33	6 - 45	9.86e-18	6.16e-12
TSw34	6 - 10	3.07e-17	4.01e-12
TSw35	60 - 71	7.51e-18	6.95e-12
TSw36	90 - 106	9.15e-17	4.01e-12
TSw37	18 - 30	3.24e-17	4.01e-12
CH1vc	25 - 30	1.57e-12	7.24e-13
CH1zc	25 - 30	5.62e-16	1.00e-13
CH2zc	13 - 19	2.03e-18	2.47e-13
CH3zc	42 - 52	2.03e-18	2.47e-13
CH4zc	17 - 20	5.47e-18	1.00e-13
PP3vp	25 - 50	1.01e-16	3.01e-14
PP2zp	0 - 10	6.11e-17	1.00e-13

11.6 The TOUGH2 Code and Equation of State Modules

The integral finite difference code TOUGH2 was used for all flow simulations presented in this chapter. Two equation of state modules were employed - EOS3 (Pruess, 1991) and EOS9 (Pruess and Antunez, 1995). For two-phase simulations (water and air) EOS3 utilizes as its primary variables P_{gas} , S_{gas} , and T , with air approximated as an ideal gas, and water properties obtained from steam table relations. EOS9 treats the gas as a passive phase ($P_{\text{gas}} = \text{constant}$) and thus the CPU time required for a steady-state solution is significantly less than for simulations using EOS3. At steady-state fluid distributions, S_L is nearly identical for both modules (for a detailed discussion see Forsyth et al., 1995). Because the solution time of the fully coupled two-phase flow problem employing EOS3 is dramatically reduced once S_L is close to its steady-state value, S_L is

first determined using EOS9. For all of the simulations reported in this chapter we used the equivalent continuum method (ECM), which treats flow in the matrix and fracture as a single continuum (see Chapter 6; Doughty et al., 1996).

11.7 *Evaluation of Coarse Flows From the UZ Model*

In order to justify the boundary conditions used on the submodel the steady-state fluxes surrounding it must be evaluated from simulations using the UZ model. Data from elements surrounding and incorporated within the submodel were extracted from a three-dimensional simulation (chapter 8; Wu et al., 1996) using the TOUGH2 code. Rock parameters used in this simulation were obtained by inversion using the code ITOUGH2 at an infiltration rate of 0.1 mm/year (see chapter 3; Bandurraga et al., 1996).

The region around the submodel includes nine surface elements from the site-scale model and is traversed by the nearly N-S trace of the GDF. Fluid flux vectors, plotted in three dimensions, are shown in Fig. 11.7.1 for the nine columns (each having approximately 24 layers, except the elements in the fault plane where the stratigraphy is doubled). The GDF is shown as a red plane, the approximate location based on the UZ model fault element node positions. The outline of the interior submodel domain (to be described in the following sections) is also plotted. The coordinates of the X and Y axes were shortened for plotting purposes and can be easily converted to Nevada state plane coordinates (X+171000, Y+232000). All plots shown in this chapter are referenced to this same set of coordinates.

Figure 11.7.1

Liquid flux vectors from UZ model simulation in area around submodel domain. Filled circles are UZ model grid nodes projected onto the base. The red plane represents the approximate geometry of the Ghost Dance Fault, as indicated by the UZ model fault element nodes. The inner submodel domain is shown as the rectangular box. The strong lateral flow in the vitric layers CH1vc (elevation ~900m; south-trending) and PP3vp units (elevation ~790 m; north-trending) is substantially greater than in all other units.

The highest fluid fluxes are within vitric layers (UZ model hydrogeological units CH1vc and PP3vp) that overlie low permeability zeolitized layers of the Calico Hills and Prow Pass units. The upper Calico Hills vitric layer (CH1vc) lies directly below the Topopah Spring unit (TSw) and overlies a low permeability zeolitic unit (CH2zc), whereas the PP3vp layer is sandwiched between zeolitic horizons. In both of these vitric horizons the flows are nearly horizontal, trending south in the CH1vc (~890m) and north in the PP3vp unit (~775m). The flow paths follow the general direction of the strike of the contact between the western vitric portion of the CH1vc and the zeolitic zone to the east (CH1zc). The much lower permeability zeolitic zone is a barrier to flow in this region.

Because the fluid fluxes in the Topopah Spring unit are several orders of magnitude lower than in the underlying Calico Hills vitric units the latter data points were removed and the flux vectors rescaled. Flux vectors in the TSw (~900-1200m) are predominantly vertical downward and several orders of magnitude lower than in the underlying vitric units (Fig 11.7.2). There is some south-trending flow in the Tiva Canyon unit (~1275m: TCw) and the Paintbrush unit (~1200-1250m: PTn) that is not as strongly developed within the center of

the submodel domain. At the infiltration rate of 0.1 mm/yr liquid, fluxes for the two fault elements are relatively small and diminish downward owing to capillary suction into the surrounding matrix. The contrasts with observations of bomb pulse ^{36}Cl in water associated with faults at the repository level in the ESF (Fabryka-Martin et al., 1996).

Figure 11.7.2

Renormalized liquid flux vectors for TSw, PTn, and TCw units from UZ model simulation in area around submodel domain. Strong lateral flow is evident in the PTn, while flow in the TCw and at the level of the ESF (about 1085m) is predominantly vertical. Fluxes along the fault diminish with depth, owing to the higher capillary suction of the surrounding matrix.

Normalizing the vertical flux by the infiltration rate gives an indication of the possible loss or gain of fluid through channeled infiltration. Fig 11.7.3 (a) shows a column of the normalized vertical flux components taken within the submodel domain (element 185 in the UZ model). For the entire repository horizon and (~1085m) TSw unit the ratio is approximately one, with a very sharp and substantial positive deviation in the Prow Pass vitric unit, as shown previously in the three-dimensional flux vector diagram (Fig. 11.7.1). At the approximate level of the ESF (~1085m), for a grid node within the submodel domain, the magnitude of the percolation flux is 0.155 mm/yr -- about 50% higher than the infiltration rate (see section 9 below). The proportion of the vertical flux (here negative in the downward direction) to the magnitude of the flux is shown in Fig. 11.7.3 (b) for the same column. As expected the vertical component of the flux is near zero in the Prow Pass unit and also in the Calico Hills vitric unit where the flows are horizontal. Within the TSw, the ratio is nearly

everywhere -1.0, indicating that the flux is near vertical throughout the unit. Near the surface, in the TCw, there is also a nonvertical flux component and less so in the PTn. From the earlier three-dimensional vector flux diagram (Fig. 11.7.2) the lateral components of flow in the TCw and PTn in the submodel area are less than in the region to the west and northwest in the UZ model. Although the UZ model does not indicate a substantial impact of the lateral flows on the TSw unit, it may become important in the vicinity of a fast flow path through the PTn.

Figure 11.7.3

The vertical component of the fluid flux from element 185 in the UZ model normalized to the 0.1 mm/yr infiltration flux (a) and the magnitude of the flux (b).

In general, the mostly vertical flow paths in the UZ model at the repository level supports our choice of a submodel in this area. The nonvertical flows in the overlying PTn and TCw units suggests that we should include a larger region above the submodel domain to capture the effects of these lateral fluxes. Even with the lateral flow in the overlying units, the ratio of the percolation flux at the repository horizon to the local infiltration flux is close to one, indicating that the lateral fluxes do not substantially modify the total flux in the TSw. Because of the regional confined lateral flows in the CH1vc and PP3vp vitric units, the submodel in its present form cannot predict the larger-scale transport of fluids after passing through the base of the TSw.

11.8 Development of the UZ Submodel

11.8.1 Numerical Grid

A three-dimensional submodel of the UZ model was created with square 10 x 10 meter elements (in plan view) having dimensions of 16 elements (E-W) by 10 elements (N-S) and 24 layers (Fig. 11.8.1). The western boundary of the model is bounded by the position of the ESF and the eastern boundary is taken close to the trace of the Ghost Dance Fault. The northern boundary is approximately that of the North Ghost Dance Fault Alcove, whereas the southern boundary is set 100 meters to the south. This regular grid was then surrounded by coarse grid elements to minimize local boundary effects and to capture some of the regional nonvertical flow in the overlying PTn and TCw units. The number of grid elements is 5846, plus 250 bottom boundary elements in all simulations, and an additional 250 top elements for simulations employing the EOS3 module.

Figure 11.8.1

Plan view of submodel grid showing inner rectangular mesh and coarse outer mesh. Positions of the ESF and GDF from the UZ model are the approximate bounds to the inner submodel (blue box).

Near-surface flow in the overlying TCw unit deviates from the horizontal, apparently controlled mostly by topographic variations. Because of some regional lateral flow in the PTn, the downward fluid flow to the repository horizon in the submodel may be slightly lower than the UZ model would predict, although as we showed in the previous section this effect was not evident at this location. To account for such possible effects, and to remove the numerical

boundaries away from the submodel boundaries, coarse grid elements were added in the upstream and downstream directions (ascertained from the UZ model).

Unit thicknesses were derived from the same isopach thickness data used to generate the UZ model input data (see Table 1). Some modifications to unit designations (TSw32 and TSw33) were made because of apparent discontinuities resulting from the coarse scale of the vertical discretization relative to the X and Y internodal distances and the dip of the units. Because a boundary exists between the regions of the Calico Hills unit that are either zeolitic or vitric (CH1zc and CH1zc), the elements at the boundary were assigned based on their areal overlap. This boundary crosses the outer coarse grid region, to the west of the inner rectangular submodel domain. The lowermost unit in the western part of the submodel is PP2zp, however because of its approximately eastward dip below the water-table, on the eastern side the lowermost unit becomes PP3vp.

11.8.2 Initial and Boundary Conditions

The dominantly vertical flow in the TSw unit indicates that the lateral boundary conditions of a submodel enclosed within this zone may be set to no mass flux and free slip. For purely vertical flow this is equivalent to a condition of lateral continuity. The upper boundary condition was set to a spatially uniform and constant infiltration rate for two different cases (0.1 mm/yr and 5.0 mm/yr). The gas pressure at the surface is given an initial value of 90 kPa, which is allowed to equilibrate to a steady-state profile, assuming a fixed lower boundary gas pressure. The lower boundary condition (at the water table) was set to a constant gas pressure ($P_{\text{gas}} = 92$ kPa) with practically full liquid saturation ($S_L = 0.999$). For simulations coupling energy conservation as well as mass conservation the surface temperature was set to a uniform and constant 17 deg. C and the temperature at the base of the submodel was set to 30 deg. C, based on UZ thermal models (chapter 9: Wu et al., 1996). The specific enthalpy of infiltration water was set to a constant 75.61 kJ/kg (chapter 9: Wu et al., 1996; chapter 12: Finsterle et al., 1996).

11.9 Numerical Simulations

In this section we describe a series of steady-state simulations employing the submodel described above. These simulations were designed to determine the local percolation fluxes at the repository horizon for constant infiltration rates and to compare these higher resolution results to those obtained from the much coarser grid UZ model. The fluxes observed in the submodel simulations using the UZ model geologic properties are then compared to simulations in which the permeabilities are modified by a stochastic field generated by simulated annealing.

11.9.1 Steady-State Liquid Fluxes, Saturations and Temperature Gradients

Steady-state simulations were performed using areally uniform infiltration rates of 0.1 and 5.0 mm/year. A rate of 0.1 mm/yr is suggested from the inverse modeling of matrix properties (see chapter 2; Bandurraga et al., 1996). The much higher value of 5.0 mm/yr is the approximate value obtained from the infiltration map of Flint et al. (1996) at the surface location above the proposed percolation flux test area. Mapped onto the UZ model grid, the infiltration rates show spatial differences of more than an order of magnitude over less than 100 meters and between neighboring grid nodes (Fig. 11.9.1). The high local variability in the infiltration rates at the scale of the submodel make any values extracted from this local data set uncertain. Therefore, simulations were performed using the two bounding rates to evaluate the likely range of percolation fluxes at the repository horizon.

Figure 11.9.1
Infiltration rates at UZ model grid nodes, as derived from Flint et al., (1996). Fluxes to the south of the submodel domain (inner grid) are up to 20 times higher than those to the north.

Steady-state flux vectors for the inner rectangular submodel domain are shown in Fig. 11.9.2 for an infiltration rate of 0.1 mm/yr. Very strong down-dip layer-parallel flow is pronounced in the upper PTn unit, with a maximum absolute flux of about 1.12 mm/yr, over 11 times greater than the infiltration flux. Some lateral flow is also evident in the vitric Calico Hills unit, but only about a third that observed in the PTn. Much lower fluxes are observed in the Topopah Spring unit, and some deviations from the vertical are evident at the base of the repository horizon.

Figure 11.9.2

Steady-state fluid flux vectors for an infiltration rate of 0.1 mm/yr. Strong lateral flow (maximum = 1.12 mm/yr) is evident in the PTn (elevation ~ 1230 to 1238 m).

At the eastern boundary of the submodel the flow in the PTn and below is diverted downward as a result of the no-flux condition (Fig. 11.9.3). As this is also the approximate position of the Ghost Dance Fault, and if the fault is acting as a impermeable barrier, then this boundary condition may be reasonable in the sense of the larger scale flow. However, even if the fault is acting as a barrier because of the offset of more permeable units, the high permeability of the fault would act as a better conduit than the submodel boundary conditions allow (in their present form). Alternatively, capillary suction in the rocks adjacent to the fault would keep the fault relatively dry and thus flow would be distributed preferentially in the matrix as the UZ model indicates. The offset of the PTn at the GDF is apparently complete (Fig. 11.5.1) suggesting that flow would either be diverted down the fault fractures or in the adjacent rock matrix (in contrast to the ^{36}Cl findings).

Figure 11.9.3

Flux vectors for the upper TSw layer to the bottom of the TCw unit (partial layer on east side). The strong lateral flows are in two of the thin upper PTn units. Lateral flows are directed vertically downward near the contact of the eastern boundary. Flux magnitude contours projected onto the base are of the lowermost layer (top TSw unit).

Even though the lateral fluxes in the PTn are quite high, the fluxes in the underlying TSw layers are predominantly vertical and much closer to the 0.1 mm/yr infiltration rate (Fig. 11.9.3). The flux contours shown in this figure are for the uppermost layer of the TSw (the lowermost layer in the section plotted). As the flux vectors indicate, the fluxes are much higher as the eastern boundary is approached, but only about a factor of two higher than the infiltration rate, much lower than the factor of over 11 seen in the PTn.

The major proportion of fluid is transported by the matrix, because of the low fracture porosity ($\sim 2 \times 10^{-4}$) and the typically low saturations of water in fractures. The fluid distributions are dependent on the values of the van Genuchten parameters chosen, which is treated in detail by Wu et al. (1996) (see Chapter 8, Wu, 1996).

Just above the level of the ESF, and near the top of the repository horizon (1094 m) the fluxes are also much higher adjacent to the eastern boundary, yet the effect has diminished somewhat and some local variations are evident (Fig. 11.9.4). Two factors contribute to the higher fluxes near the eastern boundary at this level. First, as was shown for the PTn and upper TSw layer, the flow is diverted downward at the eastern boundary. Second, the rock properties change at this level (TSw34 at the west and TSw33 at the east) because of the

Submodel of Percolation Flux at the Repository

eastward dip of the units. The permeability of TSw33 is about an order of magnitude higher than TSw34 and thus one would expect flow to be enhanced preferentially in the eastern zone. Liquid saturations differ across the submodel at this same level with higher values near the eastern boundary, but also at the western boundary also reflecting the combined effects of local rock property variations and flux differences (Fig. 11.9.5).

Figure 11.9.4

Contour map of the flux vector magnitudes for layer (TSw34-TSw33) at approximately the 1094 meter level, for an infiltration rate of 0.1 mm/yr.

Figure 11.9.5

Contour map of liquid saturations for layer (TSw34-TSw33) at approximately the 1094 meter level, for an infiltration rate of 0.1 mm/yr.

Results obtained using an infiltration rate of 5.0 mm/yr exhibit similar flux patterns to the 0.1mm simulation, with some differences owing to locally higher saturations. Flux magnitude contours at same level as in Fig. 11.9.4 (~1094m) also show the higher fluxes at the eastern boundary, yet they are only about 30% higher than the infiltration rate as opposed to 90% for the 0.1 mm/yr case (Fig.11.9.6). Liquid saturations at this level (Fig. 11.9.7) are about the same for the eastern boundary as in the 0.1 mm/yr case (~ 0.80 to 0.82). At the western boundary, however, the saturation is much higher at the 5.0 mm/yr infiltration rate (0.95 compared to 0.85).

Figure 11.9.6
Contour map of the flux vector magnitudes for layer (TSw34-TSw33) at approximately the 1094 meter level, for an infiltration rate of 5.0 mm/yr.

Figure 11.9.7

Contour map of liquid saturations for layer (TSw34-TSw33) at approximately the 1094 meter level, for an infiltration rate of 5.0 mm/yr.

In addition to the higher fluid fluxes associated with an increased infiltration rate, there is also an associated thermal effect from the downward advection of cooler surface fluid. The assumed boundary conditions (approximate values from the UZ model) are 17 deg. C at the surface and 30 deg. C at the water table and the base of the simulation. Steady-state temperature profiles for infiltration rates of 0.1 mm/yr and 5.0 mm/yr are shown in Fig. 11.9.8, taken from one column in the center of the inner rectangular simulation subdomain. There is small but noticeable cooling effect at the higher infiltration rate throughout the rock column. The differences in the temperature gradients are greatest near the surface (0.1mm/yr > 5.0 mm/yr), and decrease with depth until about the 1000m level where they are same. Below this depth the 5.0 mm/yr infiltration rate profile has a larger gradient than the 0.1mm/year profile, as a result of the constant temperature lower boundary condition. At the approximate level of the ESF (1085 m) the local temperature gradient (dT/dZ) is about 0.34 deg C/km lower for the higher infiltration rate of 5.0 mm/yr (Table 11.9.1). The fluxes at this location are somewhat higher than the infiltration rate, so that in areas where the local fluxes are different (i.e., near the eastern and western boundaries) the effect would be correspondingly larger or smaller.

Figure 11.9.8.

Steady-state temperature profiles from center of submodel domain for infiltration rates of 0.1 and 5.0 mm/yr.

Table 11.9.1 Steady-State Conditions at Repository Horizon For Differing Infiltration Rates		
	0.1 mm/yr	5.0 mm/yr
dT/dZ (deg. C/km)	17.48	17.14
Liquid Saturation	0.87	0.95
Vertical Fluid Flux (mm/yr)	0.127	5.396

Overall, the results of the steady-state submodel simulations shows that small-scale differences in fluxes can be significant, at a scale smaller than the UZ model can describe. This becomes even more significant, considering that the rock properties used in the submodel were extracted from the UZ model and do not reflect the local heterogeneities invariably present. The boundary conditions of the submodel affect the fluxes considerably, and thus the influence of the Ghost Dance and Sundance Faults on fluxes and saturations at the scale of the submodel should be investigated further. Even with these boundary effects, the fluxes at the repository horizon are predominantly vertical, in agreement with the UZ model. In the following section we can make a more detailed comparison of the UZ model and submodel at the repository horizon.

11.9.2 Comparison to UZ Model Results

It is useful to compare the results of the steady-state fluxes in the submodel to UZ model simulations. One element from the UZ model has its nodal position within the interior subdomain of the submodel and simulation results from this element (see chapter 8: Wu et al., 1996) are compared to the average of all nodes in the interior submodel domain (216 nodes) at the approximate level of the ESF (1085 m). Table 11.9.3 lists the temperature, water saturation, and the fluid flux for each model simulation. While there are some differences, the fluxes in the UZ model are only 12% higher than the average submodel flux, and both are higher than the infiltration rate. Given that the coarseness of the UZ model is about 10 times greater than the submodel, and the bounds of the UZ model element do not directly overlie the submodel, the values are reasonably close. The liquid saturation in the UZ model is significantly higher than in the average submodel, however comparison to the saturations near the same nodal position shows a closer match (0.85 to 0.87), compared to the submodel average of 0.82.

Table 11.9.2
Comparison of UZ model and Submodel at the Repository Horizon (0.1 mm/yr infiltration rate)

	UZ Model	Submodel Average
Liquid Saturation	0.91	0.82
Fluid Flux (mm/yr)	0.155	0.137

Another comparison can be made to simulations performed by Xiang et al. (1995) on a nearby column of rock, also using TOUGH2. Using three sets of rock property data (LBL, an averaged set of LBL data, and Wilson et al., 1994) they showed the water saturations, fluid velocities, and travel times at different infiltration rates. For all 3 data sets, the pore liquid velocity at about the 1085 m level was approximately 2.9×10^{-11} m/s (corresponding to 0.1 mm/yr), close to the values obtained in the submodel and UZ model simulations.

Although strong lateral flow is not observed in the CHn in the submodel simulations, the strong downdip flow in the PTn observed in the submodel is also seen in the UZ model (Chapter 9: Wu et al., 1996). Compared to the submodel, stronger lateral flow developed in the TCw unit in the UZ model, most likely a result of topographic effects and the large thickness variations in this unit.

11.9.3 Development of a 3D heterogeneous permeability field

Rock matrix heterogeneity and differences in fracture size, spacing and connectivity will lead to variations in the percolation flux at differing scales. The assessment of spatially and temporally variable fluid fluxes at a scale of tens of meters is not possible with the UZ model, because the grid elements have a horizontal length-scale of about 100 meters. Thus, the submodel can help quantify such local, but potentially significant perturbations to the flow field. Because the three-dimensional pattern of heterogeneity at the scale of our grid elements (10

x 10 meters) in the area of study is unknown, one way in which to assess the possible effects of permeability heterogeneities is to introduce stochastic variation.

Heterogeneities were imposed on the system by modification of the existing matrix and fracture permeabilities using an isotropic three-dimensional field obtained by simulated annealing (code SIMAND3D, S. Finsterle and A. Datta-Gupta, pers. comm.). Simulated annealing has previously been used for creating models of three-dimensional fracture networks (Long et al., 1991) with a final configuration close to the percolation threshold (Sahimi, 1993). Another method used to introduce small-scale stochastic heterogeneities in models of the repository horizon at Yucca Mountain is the "turning bands method" (Antunez and Pruess, 1994; Pruess and Antunez, 1995). The latter method was used to generate a distribution of fracture apertures with correlation lengths at the sub-meter scale.

Using SIMAND3D, a range of isotropic permeabilities having a standard deviation of 1.0 was generated around a hypothetical mean value (K_m) with absolute bounds three orders of magnitude around the mean. In comparison, the range of permeabilities (measured by air injection) at the repository horizon in the vicinity of the thermal alcove (TSw2) differ by three orders of magnitude over distances of a few meters (Y. Tsang, pers. comm.). Although the submodel does not have the resolution required to model heterogeneities at the scale of a few meters, it is not clear from the thermal alcove measurements whether these small-scale features do not have some larger scale connectivity or aggregation as might be expected.

The dimensions of the heterogeneities created by the simulated annealing process are controlled by the lengths over which smaller-scale variations may be correlated. The correlation lengths were set to 100 meters in the X and Y directions, and to 200 meters in the Z direction (Table 11.9.3). This choice was governed by the necessity to create heterogeneities of a plan view scale larger than a single grid element and with sufficient vertical connectivity to allow for local flow channeling. Yet the vertical connectivity was not intended to be such that the structures are continuous through the entire domain in the sense of a fault or fracture zone. The SIMAND3D code requires that the distances between vertical grid nodes are uniform. For simplicity, the vertical heterogeneities were applied directly to the nonuniform submodel grid. The end result is that correlation lengths for the vertical heterogeneities differ according to the difference in thickness between the submodel layer and 20 meter layer thickness chosen in the simulated annealing calculation. Although the correlation lengths are similar in scale to the submodel horizontal dimensions, the observed structures are typically several tens of meters in diameter, which is large enough to be properly realized using the 10m horizontal grid spacing, yet small enough such that a few full structures are observed in plan view.

Submodel of Percolation Flux at the Repository

Table 11.9.3
Spatial Parameters Used in Simulated Annealing

Coordinate	Layers	Layer Thickness	Correlation Length
X	18	10 meters	100 meters
Y	12	10 meters	100 meters
Z	24	20 meters	200 meters

Dividing the generated permeabilities (κ_s) by the hypothetical mean value (κ_m) gives the factor which was then applied to the UZ model permeabilities (κ_{UZ}) to obtain the new permeability field. Thus the modified permeability field ($\bar{\kappa}$) used in the simulations is given by:

$$\bar{\kappa} = \frac{\kappa_{st}}{\kappa_m} \kappa_{UZ} \quad (11.4.1)$$

The ratio of the vertical to horizontal permeability from the UZ model was maintained constant. The stochastic variations were generated only for the interior regular grid, so that the permeabilities of the surrounding coarse grid elements were left unchanged, thus minimizing focused nonvertical flow in the boundary elements. The contoured permeability field is shown on an E-W cross-section through the center of the submodel domain (Fig. 11.9.9) and as a horizontal slice taken close to the level of the ESF (Fig. 11.9.10). There is obvious horizontal and vertical connectivity of the generated structures, with inlayer variations of about 2 orders of magnitude higher and lower than the original permeabilities. This compares to a modification to the permeability field of about 2 orders of magnitude by Pruess and Antunez (1995).

Figure 11.9.9

Permeability contours for an E-W cross-section through center of submodel domain. The variations within each layer produced by the application of the stochastic field are evident as is the initial larger variation between layers.

Figure 11.9.10

Permeability contours for the TSw34-TSw33 layer (approximately 1094m elevation), near the top of the repository horizon.

**11.9.4
Steady state results for
heterogeneous permeability
field**

Two simulations were performed to investigate the steady-state saturations and fluid fluxes for a locally heterogeneous permeability field generated by application of the stochastic field to the UZ model permeabilities. For these simulations a version of TOUGH2 was used which allows for the modification of the permeability at each grid element, as described by Pruess and Antunez (1995). As in the latter study, we used the equation of state module EOS9 (described in section 6). The temperature was set to isothermal conditions (25 deg. C). Simulations were performed using the same boundary conditions and rock properties as in the previous section for infiltration rates of 0.1 mm/year and 5.0 mm/year. In reality, the infiltration rates at the surface may differ spatially because of permeability variations, however given the small-scale variations in infiltration rates shown by Flint et al. (1996), a modification of the infiltration rates locally cannot be justified at this time. In addition, at the depth of the repository such local effects are likely to be minimal because of the high permeability of the overlying PTn and the subsurface equilibration of fluid potentials. For this problem, it is assumed that the fracture and matrix van Genuchten parameters are identical to the unmodified permeability field. If matrix permeability variations are related primarily to differences in matrix pore throat radii, and likewise fracture permeabilities are primarily a function of aperture, then capillary pressures would be much different. Yet, differences in fracture connectivity and densities leading to such permeability variations would not similarly affect these parameters. Air permeability tests in the TSw at the repository horizon (Y. Tsang, personal communication) have not shown a relationship between the fracture size or density and the air permeability.

Steady-state fluid flux vectors using an areally uniform infiltration rate of 0.1 mm/year show complex flow behavior in many regions of the submodel, but are especially well developed in the PTn and CHn units. Because of the large variations in fluxes and their variable orientation throughout the submodel it is instructive to examine the fluxes in a selected location. Comparison of the fluid flux contours at the level of the proposed repository (Fig. 11.9.11) show differences from the model using the unmodified permeabilities (Fig. 11.9.4). There are some localized features of higher and lower fluxes and the overall differences are greater, yet even though the permeability variations at this level vary by several orders of magnitude the highest fluxes are only about 35% higher than in the unmodified submodel. Liquid saturations (Fig. 11.9.12) are little different in the heterogeneous submodel compared to the unmodified submodel (Fig. 11.9.5). Thus, the local deviations in permeability we imposed on the system do effect the patterns of the heterogeneities but the flux magnitudes and saturations are not as strongly modified at this level. This agrees with the study of Xiang et al. (1995) which showed similar fluid velocities at the repository horizon for columns having different overlying rock properties and modeled saturations. Of course, preferential pathways in the heterogeneous model would tend to allow greater channeling of fluid during transient events of increased infiltration flux.

Figure 11.9.11

Contour map of fluid flux magnitudes at the TSw33-TSw-34 layer (1094m), for an infiltration rate of 0.1 mm/yr. A locally higher flux region is apparent in the center of the domain, which is absent in the unmodified submodel (Fig. 11.9.4).

Figure 11.9.12.

Contour map of liquid saturations at the TSw33-TSw-34 layer (1094m), for an infiltration rate of 0.1 mm/yr. The values and patterns differ little from the unmodified saturations at this level (Fig. 11.9.4).

Submodel of Percolation Flux at the Repository

At an infiltration rate of 5.0 mm/yr, the local perturbations of fluid vectors are enhanced relative to the 0.1 mm/yr simulation. It is most evident in the PTn (Fig. 11.9.13) and in the CHn. In the PTn a near vertical fast flow path about 100 meter high developed in the west side of the domain that passes directly into the top of the TSw. It is about 30 meters in diameter and most of the flux is transmitted through two elements. Contours of the fluxes in the TSw, projected onto the base of the figure, show strong variations in fluxes, but clearly attenuated compared to the fluxes in the PTn. Even so, the fluxes are locally up to 20 mm/yr, a factor of four higher than the infiltration rate. Other less well-defined paths are also evident in the east side of the domain. Another aspect of the increased channeling of fluxes through heterogeneities in the PTn is that there is less fluid reaching the eastern boundary and diverted downward. Extrapolated to the conditions near a fault, the fluxes reaching the fault would be correspondingly less.

Fig. 11.9.13.

Flux vectors for the base of the TCw, the PTn and uppermost two layers of the TSw, at an infiltration rate of 5.0 mm/yr. Locally strong fluxes in the PTn are channeled into permeability highs and into the TSw. The flux contours are for the lowermost layer shown (TSw32) and projected onto the base of the diagram.

Again, near the top repository horizon (about 1094 m) patterns of flux variations are quite evident (Fig. 11.9.14), but their magnitudes have diminished relative to those seen in the TSw just below the PTn. The values of the liquid saturations are affected little (Fig. 11.9.15), yet in the region of increased percolation fluxes they are correspondingly higher.

Figure 11.9.14
Contour map of fluid flux magnitudes at the TSW33-TSW-34 layer (1094m), for an infiltration rate of 5.0 mm/yr.

Figure 11.9.15
Contour map of liquid saturations at the TSW33-TSW-34 layer (1094m), for an infiltration rate of 5.0 mm/yr.

Although we do observe some local channel structures, there does not seem to have developed the dendritic or plume-like saturation fronts observed in the simulations by Pruess and Antunez (1995). In contrast to the latter study, the stochastic heterogeneities we applied to the permeability field are of a much

smaller magnitude than the original differences between hydrogeological units. Another difference is in the ratio of the correlation length scales of our heterogeneities to the length-scale of the simulation domain which is close to one, compared to about 0.01 for the Pruess and Antunez (1995) simulations. This would suggest that if such permeabilities were present over a large area of the UZ model, and if it had a spatial resolution on the order of 10m, we may also observe larger-scale features having local perturbations of the kind observed in our simulations.

As would be expected, permeability variations of a couple of orders of magnitude imposed on the UZ model led to variations in the local fluxes and flow patterns. However, because of the predisposition of the PTn to channel larger fluxes downdip in the submodel, the presence of local heterogeneities acted as near-vertical "drains" for this already magnified flux.

As these are steady-state results, the variations may be substantially amplified during transient events and as locally high saturations would further modify the percolation fluxes. At the level of the repository, some attenuation of the flux variations has weakened the strong differences seen in the PTn and the top of the TSw, yet significant variations still persist. Liquid saturations are little affected, yet this may be expected because the porosities were left unmodified.

Such local variations in permeabilities may either tend to have an accumulative effect on the larger-scale flow patterns or be "averaged out". Yet the proximity of such structures to faults and areas of higher infiltration rates may create strong local disturbances in the flow patterns and fluxes into the repository.

11.10 Summary

A submodel in which to investigate mass fluxes at the repository horizon was chosen near the location of the North Ghost Dance Fault Alcove, between the ESF and the Ghost Dance Fault. The three-dimensional submodel spans 160m E-W by 100m N-S and has 10m square grid elements (in plan view) with variable thicknesses derived from the UZ model. Analysis of flux vectors from a three-dimensional UZ model simulation (chapter 9: Wu et al., 1996) showed that around the submodel site fluxes are predominantly vertical at the level of the proposed repository, although significant horizontal flow exists in the underlying CH1vc and PP3vp units, and less so in the TCw and PTn.

Steady-state simulations were performed using TOUGH2, at infiltration rates of 0.1 mm/yr and 5.0 mm/yr to give bounds to the likely percolation fluxes at the repository horizon. It was found that the eastward dip of the highly permeable PTn unit allowed strong lateral flow which was subsequently diverted downward at the impermeable eastern boundary of the submodel. As this is also the approximate position of the trace of the Ghost Dance Fault and

because the offset of the PTn may be nearly complete in this area, the flow observed may be analogous to the effect of the fault. At the level of the repository, fluxes are in general near-vertical and liquid saturations are directly correlated with variations in rock properties and to a lesser degree, the flux magnitudes. While the saturations and fluxes were higher for the 5.0 mm/yr infiltration rate the overall flow patterns were similar. Comparison of 0.1 mm/yr infiltration rate results from the submodel (average over a layer at the repository horizon) and from a large element in the UZ model showed a difference of only 12% in the flux with liquid saturations and fluxes higher in the UZ model. Because the submodel can account for smaller spatial scale differences in rock properties and flow phenomena, these differences highlight the importance submodel-scale simulations.

A three-dimensional stochastic permeability field was generated using simulating annealing (SIMAND3D code) and used to modify the UZ model permeabilities (fracture and matrix). The porosity and other rock parameters were left unchanged. Simulations were performed using TOUGH2 (also at infiltration rates of 0.1 and 5.0 mm/yr) to investigate the spatial characteristics of fluxes and saturations at the repository horizon. Permeability heterogeneities increased the variations in fluxes at the repository horizon, but saturations were little changed because they are a stronger function of the porosity and capillary pressure differences. In the Paintbrush and Calico Hills units several vertical "fast paths" developed that were several tens of meters in diameter and about 100 meters long. The strong lateral (down dip) flow in the PTn was subsequently channeled into these local permeability highs, resulting in fluxes a factor of four higher in the upper layers of the TSw.

We consider the results and conclusions expressed in this chapter to be scientifically valid, although they are non-Q.

11.11 References

- Antunez E. and K. Pruess, The use of the turning bands method (TBM) to generate stochastic aperture distributions in heterogeneous fractures, Lawrence Berkeley Laboratory Report LBL-35581, Lawrence Berkeley Laboratory, Berkeley, CA, 1994.
- Birkholzer, J.T., C.F. Tsang, Y. Tsang, and J.S.Y. Wang, Drift scale modeling, Yucca Mountain Milestone T6540, Scaling and modeling testing for use in TSPA, Sandia National Laboratory, Albuquerque, NM, 1996 (preliminary.)
- Fabryka-Martin J.T., P.R. Dixon, S. Levy, B. Liu, H.J. Turin, and A.V. Wolfsburg, Summary report of chlorine-36 studies: systematic sampling for chlorine-36 in the Exploratory Studies Facility, Los Alamos National Laboratory Milestone Report 3783AD (Level 4), Los Alamos National Laboratory, Los Alamos, NM, 1996.

Submodel of Percolation Flux at the Repository

- Flint A.L., J.A. Hevesi, and L.E. Flint, Conceptual and numerical model of infiltration for the Yucca Mountain area, Nevada, U. S. Geological Survey Water Resources Investigation Report, U. S. Geological Survey, Denver, CO, 1996.
- Forsyth P.A., Y.S. Wu, and K Pruess, Robust numerical methods for saturated-unsaturated flow with dry initial conditions in heterogeneous media, *Advances in Water Resources* 18, pp. 25-38, 1995.
- Hudson D.B. and A.L. Flint, Estimation of shallow infiltration and presence of potential fast pathways for shallow infiltration in the Yucca Mountain area, Nevada, U.S. Geological Survey Water-Resources Investigations Report, U. S. Geological Survey, Denver, CO, 1996 (in review).
DTN GS960508312212.006 Non-Q
- Long, J.C.S., K. Karasaki, A. Davey, J. Peterson, M. Landsfeld, J. Kemeny, and S. Martel, An inverse approach to the construction of fracture hydrology models conditioned by geophysical data, *Int. J. Rock Mech. Min. Sci. Geomech. Abstr.*, 28, pp. 121-142, 1991.
- Pruess K., TOUGH2-A general-purpose numerical simulator for multiphase fluid and heat flow, Lawrence Berkeley Laboratory Report LBL-29400, Lawrence Berkeley Laboratory, Berkeley, CA, 1991.
ACC# NNA.19940202.0088
- Pruess K. and E. Antunez, Application of TOUGH2 to infiltration of liquids in media with strong heterogeneity, *Proceedings of the TOUGH Workshop '95*, Lawrence Berkeley Laboratory Report LBL-36872, Lawrence Berkeley Laboratory, Berkeley, CA, pp. 69-76, 1995.
- Rousseau J.P., E.M. Kwicklis, and D.C. Gillies, Hydrogeology of the unsaturated zone, North Ramp area of the Exploratory Studies Facility, Yucca Mountain, Nevada, U.S. Geological Survey Water-Resources Investigations Report, U. S. Geological Survey, Denver, CO, 1996 (draft).
- Sahimi M., Flow phenomena in rocks: from continuum models to fractals, percolation, cellular automata, and simulated annealing, *Reviews of Modern Physics*, v. 65 (4), pp. 1393-1534, 1993.
- Wessel P. and W.H.F. Smith, New version of the generic mapping tools released, *EOS Trans. Amer. Geophys. U.*, v. 76, pp. 329, 1995.
- Wilson, M.L., Sensitivity analyses for total system performance assessment, In: *Proceedings of the Fourth Annual International Conference on High-Level Radioactive Waste Management*, American Nuclear Society and American Society of Civil Engineers, Eds., Las Vegas, NV, v. 1, pp. 14-21, 1993.
ACCN: NNA.19930702.0013

Submodel of Percolation Flux at the Repository

Xiang Y., S. Mishra, and B. Dunlap, Parametric analysis of a TOUGH2 model for the unsaturated zone at Yucca Mountain, Proceedings of the TOUGH Workshop '95, Lawrence Berkeley Laboratory Report LBL-37200, UC-1240, Lawrence Berkeley Laboratory, Berkeley, CA, pp. 58-68, 1995.

**SIMULATION OF COUPLED PROCESSES
IN A TWO-DIMENSIONAL
WEST-EAST CROSS-SECTION
OF YUCCA MOUNTAIN, NEVADA**

*S. Finsterle, T.M. Bandurraga, C. Doughty,
and G.S. Bodvarsson*

August 1996

12.1 Introduction

12.1.1 Importance of Coupled Processes at Yucca Mountain

Predicting flow and transport at Yucca Mountain requires a good understanding of the pertinent physical processes, their relative importance, and their interaction. In addition, knowledge about a large number of model parameters is required. In this study, we focus on the coupling of different processes, and illustrate how the combination of hydrologic and thermal effects determine liquid, gas and heat flow as well as transport characteristics. Moreover, we examine whether the conceptual model and parameter values used in the unsaturated zone (UZ) model are able to provide a consistent picture of the overall system behavior, i.e. whether the model is able to reproduce the observations made at Yucca Mountain, and whether it correctly mimics its salient features. This work provides the basis for extending coupled process modeling over the entire 3-D model domain of the UZ model.

Simulation of coupled processes requires accurate modeling of a variety of physical processes which occur on different spatial scales, are either highly transient or required to reach near steady-state conditions, involve both fracture and matrix flow and their interaction, and are sensitive to different parameters, most of which are not well known. Furthermore, parameter values optimized to explain a certain effect may contradict data which are governed by another process. For example, differences between the gas isotope ages in the Tiva and Topopah units as well as the pneumatic pressure signal require relatively low gas permeabilities for the Paintbrush unit. On the other hand, the ^{36}Cl data may necessitate fast moisture-flow path through some fractures in the Paintbrush. The attempt to explain both effects in a single model is thus a challenge. At the same time, modeling coupled processes provides an opportunity to discriminate between alternative scenarios. While a certain effect may be accounted for by more than one conceptual model, a comparison of modeling results with all available data may render certain aspects of the model unlikely. New features and parameters become relevant, such as the properties of the major faults and their offsets, boundary conditions such as variable and locally increased infiltration rates, certain geologic features such as the apparent discontinuity in the Calico Hills zeolites, etc. (see Chapter 1, Bodvarsson et al. 1996).

The simulations presented in this chapter will involve no calibration, i.e. it is assumed that the previous calibration efforts described in Chapter 3 and Chapters 7 through 10 as well as Ahlers et al. (1996) have produced a reasonable UZ site scale model. By taking a representative cross-section through the repository hori-

Simulation of Coupled Processes in a Two-Dimensional West-East Cross-Section of Yucca Mountain, Nevada

zon of the UZ model and subjecting it to comparisons with observed data of gas pressure, moisture tension, saturation, and temperature will give it a rigorous test that should reflect the robustness and conversely the limitations of the UZ model.

12.1.2 Purpose of Study

The modeling study described in this report is an attempt to reproduce and partly explain a variety of data and observations using a two-dimensional west-east cross-section of Yucca Mountain. A dual-porosity, dual-permeability representation of the fracture-matrix system will be developed for transient simulations where the resolution of the driving pressure and temperature gradients at the fracture-matrix interface is important. Multiphase flow processes under non-isothermal conditions are taken into account. A single parameter set which combines estimates from individual calibration studies is used (see Ahlers et al., 1996, as well as Chapter 3 and Chapters 7 through 10).

The objective of this effort is to demonstrate that the salient features of flow and transport at Yucca Mountain are reproduced by the unsaturated zone model. Matching observations of different types validates the conceptual model and checks the consistency of the parameter set, thus increasing the reliability of the subsequent model predictions.

Following a general description of the modeling approach in Section 12.2, we discuss a few selected process simulations and relate the results to the observed data. The observations are only briefly described; the reader is referred to the parallel reports and the literature. The processes and data considered in this study are summarized in Table 12.1.2.1.

Table 12.1.2.1 Summary of Key Processes and Affected Data		
Process	Observation	Section
steady-state flow	saturation	12.3.1
	water potential	12.3.2
	temperature	12.3.3
gas flow	gas circulation and isotope ages	12.4.2
	pneumatic pressure response	12.4.3
liquid flow and transport	liquid flow	12.5.1
	^{36}Cl pulse	12.5.2

12.1.3 QA Status of Data and Software Used in this Chapter

The simulation discussed in this chapter are based on a parameter set for rock properties derived from borehole data and inverse modeling. The QA status is described in Bandurraga et al. (1996), Chapter 3. Furthermore, we make qualitative comparisons between the modeling results and data available for

Simulation of Coupled Processes in a Two-Dimensional West-East Cross-Section of Yucca Mountain, Nevada

the cross-section under investigation. The QA status of these data is summarized in Table 12.1.3.1.

Table 12.1.3.1 QA Status of Data Used in this Chapter				
Data Type	Bore-hole	Author	DTN	QA-Status
saturation	SD-7	Flint	GS951108312231.009	Q
saturation	UZ#16	Flint	GS940508312231.006	Q
saturation	UZ-6s	Loskot	GS921208312211.013	non-Q
water potential	SD-7	Flint	GS951108312231.009	to be Q
temperature	H-3	Sass	GS930208318523.001	non-Q
temperature	UZ-7a	Rousseau	GS960308312232.001	to be Q
infiltration map	-	Flint	-	to be Q
^{36}Cl	ESF	Fabryka-Martin	-	to be Q
pneumatic data	SD-7	Patterson	-	to be Q
gas isotopes	UZ-6s	Thorstenson	-	non-Q

The data listed in Table 12.1.3.1 as "to be Q" are in the process of being qualified by the U.S. Geological Survey. The "non-Q" data do not effect the conclusions of this report.

All the simulations were performed using computer programs that underwent software qualification. The main simulation program is TOUGH2 (Pruess et al., 1996). The ECM module software qualification is described in Wu et al. (1996).

This work and its conclusions will be Q once the geological model and the data listed in Table 12.1.3.1 achieve Q status. At present, they provide strong corroborating evidence for the conclusions reached in this modeling study.

12.2 Model Development

In this chapter we briefly describe the modeling approach, discuss initial and boundary conditions and model assumptions that are common in all the following simulations.

12.2.1 Two-Dimensional Cross-Section

We have selected a vertical west-east cross-section, which starts about 1 km west of the Solitario Canyon fault, passes boreholes USW UZ-6, USW UZ-6s, and USW SD-7, intersects the Ghost Dance and Dune Wash faults, contains borehole UE-25 UZ#16, and extends about 1.5 km beyond the Bow Ridge fault to the east. The corresponding Nevada North coordinate is 231,800 m.

Simulation of Coupled Processes in a Two-Dimensional West-East Cross-Section of Yucca Mountain, Nevada

This cross-section was selected because it contains boreholes that showed various processes. borehole SD-7 has a perched water zone and rather descriptive moisture tension and saturation profiles. Borehole UZ#16 also has good quality saturation data in addition to measured ^3H concentrations in the Calico Hills units that reflect less than 40 years travel time from the ground surface. The conceptual model of the area (see Chapter 2, Bandurraga et al. 1996) identifies a vitric "hole" in the zeolitic zone of the Calico Hills formation that has potentially great implications for radionuclide transport at the site. Borehole UZ-6 and UZ-6s have very active shallow gas flows that outflow during winter and inflow during the summer. In addition, the latest infiltration map indicates large variability in average infiltration with highest infiltration at the crest of Yucca Mountain, and then declining to the east and west of this cross-section. Thus, the data associated with this cross-section provides a near-unique opportunity to investigate coupled processes involving gas, moisture, heat, and chemical transport at Yucca Mountain.

The model boundaries and layering are taken from the unsaturated zone site-scale model (Wittwer et al., 1995; Chapter 2, Bandurraga et al., 1996; Chapter 5, Haukwa et al., 1996). However, the discretization was modified, with a 50 m grid spacing in the horizontal direction and refined gridding around the faults. The mesh is shown in Figure 12.1.1 (borehole UZ-6s is not shown since is nearly coincident with UZ-6). Note the vertical exaggeration of about 6:1 in this and all the following figures.

Figure 12.2.1.1
Grid of the west-east cross-section along Nevada Coordinates N 231800.

12.2.2 Hydrostratigraphy

The hydrostratigraphy employed in the model is visualized in Figures 12.2.2.1 and 12.2.2.2 where permeabilities in the matrix and fracture continuum are shown, respectively. Figures 12.2.2.3 and 12.2.2.4 show the matrix and fracture α -parameters of the van Genuchten model. The matrix porosity field is depicted in Figure 12.2.2.5. The model consists of 23 hydrostratigraphic units and contains four faults. The hydrogeologic properties have been determined from laboratory measurements and inverse modeling, and are described in Chapter 3, Bandurraga et al. (1996). Most units are densely fractured. As shown in Chapter 6 (Doughty et al., 1996), the fracture-matrix system can be accurately represented by an Effective Continuum Model (ECM) whenever steady-state conditions prevail. The ECM model is described in Pruess and Tsang (1994) and Chapter 4 (Wu et al., 1996). For highly transient simulations, however, where changes of fluid pressures, temperatures, and phase compositions propagate rapidly through the fractures, while invading the tight matrix blocks much more slowly, fluid and heat flow from the fractures into the matrix and vice versa has to be modeled explicitly. We employ the method of Multiple Interacting Continua (MINC; Pruess and Narasimhan, 1982, 1985; Pruess, 1991). The MINC method is a generalization of the classic dual-porosity concept where fracture-matrix flow is modeled by means of one-dimensional strings of nested grid blocks. The MINC approach is more general as it allows for global flow in both fracture and matrix continua. In this study, only two continua are specified, and global fracture-fracture as well as matrix-matrix flow is considered, i.e. we use a dual-porosity, dual-permeability approach to model the fractured-porous units at Yucca Mountain.

Figure 12.2.2.1
Matrix permeabilities.

Simulation of Coupled Processes in a Two-Dimensional West-East Cross-Section of Yucca Mountain, Nevada

Figure 12.2.2.2
Fracture permeabilities.

Figure 12.2.2.3
Matrix α -parameters of the van Genuchten model.

Simulation of Coupled Processes in a Two-Dimensional West-East Cross-Section of Yucca Mountain, Nevada

Figure 12.2.2.4.
Fracture α -parameters of the van Genuchten model

Figure 12.2.2.5.
Matrix porosities.

12.2.3
Initial and Boundary
Conditions

Boundary conditions for all steady-state runs have been selected as follows. We first deal with the land surface where atmospheric conditions are prescribed. In order to arrive at elevation-dependent atmospheric conditions, a numerical, one-dimensional, gas-filled column was set up. Based on data at Yucca Crest (Thorstenson et al. 1989), an average temperature of 15.9 °C at elevation 1484 m was prescribed, and a temperature of 19.9 °C was fixed at an elevation of 1084 m, corresponding to a lapse rate of 0.01 °K/m. Gas pressure at Yucca Crest was set to 85 kPa, and relative humidity was assumed to be 20%. A high-resolution simulation to steady state was performed with a no flow boundary at the bottom, yielding a static gas pressure profile under non-isothermal conditions. The resulting pressures, temperatures, and air mass fractions were then assigned to the 2-D model according to the elevation of each boundary grid block of the cross-section.

Next, a single-phase gas simulation with the 2-D model assuming 100% relative humidity was performed, yielding gas pressures at the water table where temperature was fixed at 32 °C. The resulting pressures, which are on the order of 93 kPa, were then fixed at the bottom boundary, and saturation was set to one at the water table and 0.3 elsewhere. A variable recharge rate which is based on an infiltration map provided by A. Flint, USGS, was specified at the surface (Figure 12.2.3.1). The average flow rate over the model domain is about 3 mm/year, with regions of high infiltration up to 20 mm/year, and very small infiltration, for example, east of the Bow Ridge fault. The enthalpy of the infiltration water was assumed to be 75.6 kJ/kg, which corresponds to a temperature of 18 °C. The system was run to steady state using the ECM formulation, yielding the pressure, temperature, and saturation distribution in both the fractures and the matrix under capillary-gravity equilibrium for the assumed infiltration rate and elevation-dependent atmospheric conditions. These results are described in Section 12.3. The system state from the ECM simulation are then transferred to the corresponding MINC model. This result will be used as the initial condition for the subsequent transient runs described in Sections 12.4 and 12.5.

Simulation of Coupled Processes in a Two-Dimensional West-East Cross-Section of Yucca Mountain, Nevada

Figure 12.2.3.1

Infiltration rates applied at the surface of the model, interpolated from infiltration map provided by A. Flint, USGS.

12.3 Steady-State Conditions

In this chapter we describe the results of the steady-state simulation. Steady-state conditions are considered important since they reflect the long term behavior of the system. Most of the field data are considered to represent steady-state or near steady-state conditions. We compare the simulation results with saturation, water potential, and temperature data.

12.3.1 Saturation

The saturation and water potential data were obtained from cores and drill cuttings. The drilling and coring methods as well as the collection of drill cuttings are reported to only minimally disturb the water content of the rock (see for example Loskot (1993) and references therein). Saturation was derived by first measuring a composite gravimetric water content using oven-drying methods. Bulk- and grain-density measurements were performed to calculate porosity and eventually saturation. We compare our modeling results with saturation data from boreholes SD-7, UZ#16 and UZ-6s. More details about the data can be found in Chapter 3, Bandurraga et al. (1996).

Figures 12.3.1.1 and 12.3.1.2 show the simulated saturation distribution in the matrix and fracture continuum, respectively. In the non-welded PTn unit, where no fracture continuum exists, saturations in the two figures are identical.

Simulation of Coupled Processes in a Two-Dimensional West-East Cross-Section of Yucca Mountain, Nevada

Figure 12.3.1.1.
Simulated saturation distribution of matrix continuum.

Figure 12.3.1.2
Simulated saturation distribution of fracture continuum.

Simulation of Coupled Processes in a Two-Dimensional West-East Cross-Section of Yucca Mountain, Nevada

The saturation pattern mainly reflects the ratio in capillary strength between the fractures and the matrix, and between adjacent units. Deviations from this general observation are a result of variable infiltration rates, lateral flow diversion, and the impact of the faults. For example, elevated saturations are seen between coordinate 169.8 and 170.6 km, and again between 171.0 and 171.8 km, where higher infiltration rates are applied (see Figure 12.2.3.1). On the other hand, dryer conditions are encountered east of the Bow Ridge Fault where low infiltration rates are assigned. Furthermore, due to the west-east tilting of the layers, water tends to accumulate west of the faults until the saturation is high enough to enter the fault zone (Wittwer et al., 1995). Saturations tend to be high in the Tiva Canyon above the non-welded Paintbrush unit, in the vitrophyre layers of the Topopah Spring, and above perching layers such as the zeolites of the Calico Hills formation.

Comparisons between the calculated and measured saturation profiles in boreholes SD-7, UZ#16, and UZ-6s are shown in Figures 12.3.1.3, 12.3.1.4, and 12.3.1.5, respectively. The match is comparable to the one obtained by calibrating the one-dimensional columns (Chapter 3, Bandurraga et al., 1996).

Figure 12.3.1.3

Comparison between calculated and measured saturation profile in borehole SD-7. Data from L. Flint, USGS.

Simulation of Coupled Processes in a Two-Dimensional West-East Cross-Section of Yucca Mountain, Nevada

Figure 12.3.1.4
Comparison between calculated and measured saturation profile in borehole UZ#16. Data from L. Flint, USGS.

Figure 12.3.1.5
Comparison between calculated and measured saturation profile in borehole UZ-6s. Data from C. Loskot, USGS.

Simulation of Coupled Processes in a Two-Dimensional West-East Cross-Section of Yucca Mountain, Nevada

12.3.2 Water Potentials

Figure 12.3.2.1 shows the modeled capillary pressure distribution. The water potential in the fracture and matrix continuum are identical at steady-state due to the equilibrium assumption of the effective continuum concept. Figure 12.3.2.2 shows a comparison between the calculated and observed water potentials at borehole SD-7. The comparison is rather poor mainly due to difficulties with capillary pressure measurements at suctions near zero, and in obtaining measurements that represent in-situ conditions on the scale of a grid block.

Figure 12.3.2.1
Modeled water potential distribution.

Figure 12.3.2.2 Comparison between calculated and observed water potentials in borehole SD-7. Data from L. Flint, USGS.

12.3.3
Temperature

Following up on the discussion of results described in Chapter 9 (Bodvarsson et al., 1996), we examine the temperature gradients within our cross-sectional model and compare them to the prescribed infiltration rate. The hypothesis is that changes in temperature gradients within the unsaturated zone are primarily due to heat consumption caused by infiltration water. Geothermal heat flows upwards mainly by conduction and - to a lesser extent - convection of latent heat in the vapor phase. Part of this energy is consumed in order to bring the temperature of the downwardly percolating water into thermal equilibrium with the surrounding rock. Provided that thermal conductivity and the total heat flux is known, measuring temperature gradients is considered a means to estimate percolation flux. Furthermore, assuming that lateral flow of liquid and heat is relatively small, the estimated percolation flux can be related to the infiltration rate. This hypothesis is numerically tested using the calculated temperature distribution shown in Figure 12.3.3.1 as a synthetic data base. Recall that the model uses a variable infiltration rate, and that temperatures are kept constant at the water table and the surface. Conductive and convective heat flow is considered where the heat conductivity is a function of saturation. Consumption, transport, and release of latent heat due to evaporation, vapor flow in the gas phase, and condensation, is also taken into account. The resulting heat flow pattern is shown in Figure 12.3.3.2. We notice lower heat flow rates underneath high infiltration regions (see also Figure 12.2.3.1). Furthermore, strong perturbations can be observed within and in the immediate vicinity of the faults. Upward flow of humid air in the faults generally increases heat flow. On the other hand, condensation and generally higher saturations especially west of the faults lead to increased percolation fluxes and thus lower vertical heat flow immediately next to the faults. A more quantitative examination of temperature, heat flux and their correlation to percolation flow rates are discussed in the remainder of this section.

Simulation of Coupled Processes in a Two-Dimensional West-East Cross-Section of Yucca Mountain, Nevada

Figure 12.3.3.1
Simulated temperature distribution.

Figure 12.3.3.2
Vertical heat flux.

From the temperature distribution shown in Figure 12.3.3.1, we extract the temperature T and elevation z of the top and bottom elements of the Topopah Spring unit, and calculate the gradient $\Delta T/\Delta z$ (see Figure 12.3.3.3). No data from the faults themselves are analyzed, since they are expected to be inconsistent with the flow processes in the undisturbed tuffs. The gradients are continuous. Next, the liquid flow rate in the center of the Topopah Spring layer is used to represent percolation flux. A total of 135 simulated gradients and flow rates were evaluated along the profile. The percolation flux is then plotted against the temperature gradient (Figure 12.3.3.4). Low percolation fluxes seem to be related to higher temperature gradients, and high rates tend to be associated with low gradients, as suggested by the heat balance consideration. A regression line was fitted through the synthetic data despite considerable scattering. The regression line is very close to the theoretical one derived from a simple one-dimensional energy balance equation where the geothermal heat flux $E \approx 45 \cdot 10^{-3} \text{ W/m}^2$ is equated to the sum of conductive upward heat flow and the downward energy flux in the percolation water:

$$E = \lambda \cdot \nabla T - q_l \cdot \rho_l \cdot c_l \cdot \Delta T \quad (12.3.3.1)$$

Here, $\lambda = 1.73 \text{ W/m}^\circ\text{C}$ is heat conductivity, q_l is the volumetric liquid flow rate, $\rho_l = 1000 \text{ kg/m}^3$ is water density, $c_l = 4187 \text{ J/kg}^\circ\text{C}$ is the specific heat of liquid water, $\Delta T = 14^\circ\text{C}$ is the temperature change the downwardly percolating water undergoes as it moves from the surface to the water table. For zero and 10 mm/year percolation flux, the temperature gradient amounts to approximately 2.6 and $1.5^\circ\text{C}/100 \text{ m}$, respectively, which is consistent with the slope of the fitted line shown in Figure 12.3.3.4.

The scattering seen in Figure 12.3.3.4, i.e. the deviation of the actual percolation flux from the one predicted by the regression model, is an indication of lateral heat flux. The heat anomalies are a result of flow diversions within Topopah Spring, variable thickness of the unsaturated zone, changes in saturation leading to changes in the heat conductivity, and the impact of vertical features such as faults. Moreover, lateral heat flow is also affected by the variability in the percolation flux itself. The combined effect of the above factors leads to local temperature gradients which are not consistent with the general correlation represented by the straight line in Figure 12.3.3.4.

Figure 12.3.3.5 is an attempt to localize regions with a strong anomaly regarding the relation between temperature gradient and percolation flux. In Figure 12.3.3.5, the data points from the previous figure are connected according to the East coordinate of the sample location, so that the origin of individual data points and their position with respect to faults can be identified. We first note that the above mentioned relationship between temperature gradient and percolation flux is locally violated in many places. For example, starting at the western model boundary, the temperature gradients increase despite increasing

Simulation of Coupled Processes in a Two-Dimensional West-East Cross-Section of Yucca Mountain, Nevada

percolation fluxes. A similar behavior can be observed when approaching the Dune Wash Fault from the west. Crossing the Solitario Canyon Fault leads to a reduced temperature gradient despite an almost constant percolation flux. On the other hand, a constant temperature gradient is seen west and East of the Ghost Dance Fault despite a doubling of the water flow rate. Almost no effect of the Bow Ridge Fault can be seen which happens to be in an area of generally low and almost constant infiltration. This is remarkable because the Bow Ridge Fault exhibits a rather large offset. The differences in behavior reflect the variability of the factors that cause the anomaly. A detailed energy balance calculation including horizontal and vertical heat flow by conduction, convection, and diffusion would be extremely useful to explain the entire thermal regime at Yucca Mountain.

The regression line relating temperature gradient and percolation flux cannot be directly measured in the field. Simple one-dimensional energy balance calculations or modeling studies such as the one presented here have to be performed. Furthermore, independent estimates of heat conductivity are required. The potential error made by using a regression line for infiltration rate estimation is qualitatively depicted in Figure 12.3.3.4. We finally estimate the infiltration rate using the regression line shown in Figure 12.3.3.4 and the "observed" temperature gradients shown in Figure 12.3.3.3. We further make the assumption that liquid flow is predominantly vertical. The estimated infiltration rate using this method is shown in Figure 12.3.3.6, and is compared to the actually prescribed infiltration rate. The general pattern of relatively high and low infiltration rates is reasonably well reproduced. The average flux over the entire cross-section is about the same, a result of the straight-line fit shown in Figure 12.3.3.4. Small-scale fluctuations are not identified due to the diffusive nature of heat and fluid flow in the unsaturated zone.

We conclude that temperature gradient measurements provide a means for estimating percolation fluxes or even infiltration rates. This conclusion is based on the assumption that the linear regression model derived here is correct. It further assumes that independent estimates of heat conductivity are available, and that accurate temperature measurements in a layer of relatively uniform saturation and predominantly vertical heat and fluid flow can be made. Temperature gradients should be measured in regions that are not affected by the fault zones. A large number of temperature gradient measurements are required to obtain an integral measure of infiltration rate and its uncertainty.

The local, two- and three-dimensional effects discussed above, as well as complicated coupled heat and fluid flow processes have a relatively large impact on the temperature distribution. The actual percolation flux may be locally quite different from the one estimated with a simple regression model, as shown in Figure 12.3.3.4. Uncertainty in the input parameters should be related to the potential errors made by neglecting lateral heat flow phenomena.

Simulation of Coupled Processes in a Two-Dimensional West-East Cross-Section of Yucca Mountain, Nevada

These conclusions should be confirmed in laboratory and large-scale percolation experiments, along with three-dimensional modeling studies. A detailed sensitivity analysis is required to further assess the uncertainty of the estimated infiltration rates.

Figure 12.3.3.3

Calculated temperature and temperature gradient in Topopah Spring along the profile.

Simulation of Coupled Processes in a Two-Dimensional West-East Cross-Section of Yucca Mountain, Nevada

Figure 12.3.3.4
Calculated percolation flux as a function of temperature gradient.

Figure 12.3.3.5
Impact of faults on temperature gradient and percolation flux.

Simulation of Coupled Processes in a Two-Dimensional West-East Cross-Section of Yucca Mountain, Nevada

Figure 12.3.3.6
Infiltration rate estimated from simulated temperature gradient data, compared to actually prescribed infiltration rate.

In Figures 12.3.3.7 and 12.3.3.8, the calculated temperatures are compared to two profiles of nearby boreholes, USW H-3, and USW UZ-7a, respectively. The offset between the calculated and observed temperature profiles are mainly due to differences in the boundary conditions. Observed temperature data near the surface are affected by seasonal variations, whereas the calculated temperature near the water table is affected by the constant temperature boundary condition. Nevertheless, The temperature gradient is reasonably well reproduced.

Simulation of Coupled Processes in a Two-Dimensional West-East Cross-Section of Yucca Mountain, Nevada

Figure 12.3.3.7
Comparison between calculated and measured temperature profiles in borehole UZ-7a. Data from Rousseau, USGS.

Figure 12.3.3.8
Comparison between calculated and measured temperature profiles in borehole H-3. Data from Sass, USGS.

12.4 Gas Flow

12.4.1 Introduction

Gas flow and pneumatic pressure propagation at Yucca Mountain has been studied in detail by Ahlers et al. (1996). The gas flow pattern may provide indications regarding permeability and connectivity of faults and fractures. The gas phase has the potential to transport significant amounts of heat energy and water in form of vapor, affecting temperature and saturation distribution under both ambient conditions and after emplacement of heat-generating waste packages. Furthermore, gas and vapor flow may be an important transport mechanism for certain radionuclides such as ^{14}C and tritium.

Data reflecting gas flow at Yucca Mountain include (1) measurements of gas flow in two unlined boreholes (UZ-6 and UZ-6s) near Yucca Crest (Weeks, 1987, 1991; Thorstenson et al., 1990), (2) isotopic gas age measurements (Yang et al., 1985; Thorstenson et al., 1990), and (3) pneumatic pressure data (Rousseau et al., 1995; Patterson, 1996).

We study the gas circulation pattern assuming steady-state flow conditions and estimate gas ages (see Section 12.4.2). Response of gas pressures to atmospheric pressure changes are studied in Section 12.4.3.

12.4.2 Gas Circulation Pattern

Gas flow measurements at boreholes UZ-6s and UZ-6 have been correlated to changes in temperature, relative humidity, barometric pressure, and wind conditions near Yucca Crest (Weeks, 1987, 1991; Thorstenson et al., 1990). The boreholes continuously outflow gas during wintertime. Lower rates or even flow reversal can be observed during summertime. About 80% of the total gas flux observed at the borehole head enters the borehole in the top 30 meters (Thorstenson et al., 1990).

Several mechanisms have been identified as the driving force for gas flow near Yucca Crest (Weeks, 1987, 1991; Thorstenson et al., 1989), namely (1) topographic-induced flow due to temperature and density gradients between the air column in the atmosphere and the gas in the pore space, (2) barometric pressure changes, and (3) wind effects. We focus here on the long-term gas flow pattern as a result of thermal and topographic effects. The high influx of gas near the top of the borehole is not considered here because of insufficient resolution of that zone in the model.

Figure 12.4.2.1 shows the liquid saturation in the fracture continuum and the gas flow pattern, visualized by particle tracking. Gas flow pattern and travel times are highly sensitive to small changes in the parameters, boundary

Simulation of Coupled Processes in a Two-Dimensional West-East Cross-Section of Yucca Mountain, Nevada

conditions, and the flow dimensionality. Nevertheless, the following general observations can be made.

Figure 12.4.2.1

Calculated liquid saturation in fracture continuum and gas particle tracks. Travel time between each mark is 100 years.

Gas flow cells develop almost independently between major faults. Gas flux in the faults tends to be high and of changing flow direction, depending on its location with respect to topographic features such as depressions, slopes, or ridges. For example, the Solitario Canyon fault, which is located in a topographic low, exhibits gas intake, with a clockwise gas flow cell developing to the west and an anti-clockwise circulation cell developing to the east. This is a relatively stable flow pattern. The situation east of Yucca Crest is less stable. The topographic effect tends to induce clockwise circulation cells, with gas intake at lower elevations and outflow towards the higher elevations. However, these circulation cells are interrupted by the faults and local variations in surface elevation. The Ghost Dance fault encounters upward gas flow from the cell to its east, and tentatively downward flow to its west. Since it is located on a small topographic high, the net gas flow direction is upward. These flow patterns are likely to be changed by small daily and seasonal variations in boundary conditions.

Even under averaged annual conditions, travel times within the Tiva Canyon are relatively short, especially towards Yucca Crest, leading to gas ages less than 100 years near the surface. Wind as an additional driving force may further enhance gas circulation at shallow depths (Weeks, 1991). Note, however, that local variations may occur with relatively old gases in regions where gas flow is predominantly upward. In general, gas travel times beneath the Paintbrush unit are predicted to be much longer, on the order of 10^4 years, which is

Simulation of Coupled Processes in a Two-Dimensional West-East Cross-Section of Yucca Mountain, Nevada

consistent with the observed gas ages from isotope data (Yang et al., 1985; Thorstenson et al., 1990).

12.4.3 Barometric Pressure Response

The response to barometric pressure fluctuations at the surface was observed in specially instrumented boreholes such as USW NRG-6, USW NRG-7a (Rousseau et al., 1995), and SD-7 (Patterson, 1996). The reduction of amplitude and increase of time lag with depth was used to estimate effective gas diffusivity (Ahlers et al., 1996). It was further shown, that the construction of the Exploratory Studies Facility (ESF) has a significant effect on the observed pneumatic data, with an increase of amplitude and the appearance of a low frequency signal (Rousseau et al., 1996; Ahlers et al., 1996).

Recent data from borehole SD-7 (Patterson, 1996) cover a period before and after the construction of the ESF. In the numerical model, we prescribe the barometric pressure at the surface as a function of time, and - after the ESF is in place - also in the grid block representing the tunnel. Simulated pneumatic pressures are recorded at the depths of the sensors, and compared to the data. There is excellent agreement between the observed data (symbols) and the simulation results (solid lines) as shown in Figure 12.4.3.1.

Figure 12.4.3.1
Simulated and observed pneumatic response to barometric pressure fluctuations in SD-7.
Preliminary data from USGS (Patterson, 1996).

12.5 *Liquid Flow and Transport*

12.5.1 Liquid Flow Rates

No direct observation of liquid flow rates are available, so only simulation results are discussed in this section. In Figure 12.5.1.1, total saturation, which is close to the matrix saturation, is contoured, overlaid by a vector plot of the total liquid flow rate. Recall the vertical exaggeration of 6:1. The vertical flow component is visualized in Figure 12.5.1.2, along with vectors showing the horizontal flux component. Liquid flow is predominantly downward, and mirrors the infiltration pattern (see Figure 12.2.3.1). However, there are significant lateral flow diversions at sloping interfaces, especially on top of the non-welded Paintbrush unit, and between Topopah Spring and Calico Hills. Liquid tends to be diverted along the sloping interfaces until high saturations are built up or a fault zone is encountered. Saturation and vertical flow components are increased immediately west of a fault. It is important to realize that the flow vectors shown in Figure 12.5.1.2 represent average Darcy fluxes over the thickness of the corresponding grid blocks. Actual pore water velocities in the relatively thin water layer above perching units may be much higher. The indicated fluxes must therefore be interpreted with care, taking into account the thickness of the respective grid block, and, where horizontal flow becomes vertical, the aspect ratio of the element.

Simulation of Coupled Processes in a Two-Dimensional West-East Cross-Section of Yucca Mountain, Nevada

Figure 12.5.1.1
Total liquid saturation and liquid flow vectors.

Figure 12.5.1.2
Vertical (contours) and horizontal (vectors) flow components.

12.5.2 Fast Path

A transient dual-porosity, dual-permeability simulation of a liquid pulse has been performed to identify potential fast paths for infiltration water. The presence of a bomb-pulse ^{36}Cl signal in the ESF (Fabryka-Martin et al., 1996) implies very short travel times from the surface to the repository horizon. Fol-

Simulation of Coupled Processes in a Two-Dimensional West-East Cross-Section of Yucca Mountain, Nevada

lowing an assumed infiltration event that leads to almost fully saturated conditions in the top layers of the Tiva Canyon unit, water and environmental tracers percolate predominantly through the fault zones, but also in the fracture network, which slightly affects the saturation in the adjacent matrix blocks. Figure 12.5.2.1 shows the simulated change of liquid saturation in the fracture continuum 50 years after release of the infiltration pulse. The deepest penetration of the pulse can be observed near the fault zones and underneath regions with generally high infiltration. Water flows through the fractures to the repository horizon and reaches the elevation of the ESF. Saturation in the fracture continuum is plotted as a function of time for five locations along the profile of bore-hole SD-7 (Figure 12.5.2.2). The liquid pulse reaches the bottom of the Tiva Canyon unit almost instantly, and about 2 years are required to pass the Paintbrush unit. In this simulation, the repository horizon is reached after 30 years, and the top of the Calico Hills after about 80 years. No significant increase in saturation can be observed near the water table at the end of the simulated period of 1000 years. Note, however, that travel times through the faults are extremely short (on the order of a few weeks to reach the water table). In summary, the presence of bomb-pulse ^{36}Cl in the ESF can be explained with the current site-scale model properties, provided that fracture flow is initiated by a high infiltration event. More discussion of chemical transport at Yucca Mountain can be found in this report (Chapter 6, Doughty et al., 1996; Chapter 8, Wu et al., 1996; Chapter 10, Fairley et al., 1996; and Chapter 11, Sonnenthal et al., 1996).

Figure 12.5.2.1
Simulated change of liquid saturation 50 years after release of infiltration pulse.

Simulation of Coupled Processes in a Two-Dimensional West-East Cross-Section of Yucca Mountain, Nevada

Figure 12.5.2.2
Simulated liquid saturation as function of time in fracture continuum, near borehole SD-7

12.6 Summary and Concluding Remarks

A number of numerical simulation studies in a dual-porosity, dual-permeability model of a two-dimensional west-east cross-section have been performed. The model includes the main features currently implemented in the LBNL/USGS 3D UZ site-scale model of Yucca Mountain. A variety of coupled processes on different spatial and temporal scales have been simulated, using a single conceptual model and a single parameter set which was determined independently from data inversion studies (Ahlers et al., 1996; Bandurraga et al., 1996, Chapter 3). The modeling results were compared to observed data whenever available, or discussed in a more qualitative sense to see whether they are able to reproduce the overall system behavior according to our current understanding.

The conclusions reached in this study are based on the parameter set derived under QA standards (see Chapter 3, Bandurraga et al., 1996, and references therein). The geologic model shown in Figures 12.2.2.1 through 12.2.2.5 is not yet Q. The simulation results are compared to a number of data, the QA status of which is summarized in Section 12.1.3. This work and its conclusions will be Q once the geological model and the data listed in Table 12.1.3.1 achieve Q status. At present this data may be considered as corroborating evidence for these conclusions. We believe that the qualitative conclusions derived in this study are scientifically valid.

Simulation of Coupled Processes in a Two-Dimensional West-East Cross-Section of Yucca Mountain, Nevada

As a general conclusion, the current conceptual model of the unsaturated zone at Yucca Mountain yields predictions that are consistent with a large variety of observations. The parameters used in the model seem reasonable in the view of the existing data. Modifications have to be made if (1) local conditions deviate from the average situation, (2) the process under consideration depends on parameters that could not be accurately determined due to a lack of sensitive data, and (3) the scale of the process differs from the one for which effective parameters have been identified.

More specifically, the observed saturation distribution was reasonably well reproduced assuming steady-state conditions. The modeling results show that variations are mainly due to variations in the infiltration pattern which are not well known. A detailed model has to be set up to address the issue of perched water. Water potentials are difficult to match mainly because of large uncertainties in the data and conceptual difficulties. The model reveals the sensitivity of temperature and heat flow to the percolation flux and infiltration rate. Measuring temperature gradients across a layer of more or less constant saturation may provide a means to estimate percolation flux.

Gas flow at Yucca Mountain exhibits a complicated circulation pattern, driven by topographic and thermal gradients, and other effects such as wind forces and the impact of faults. The observed gas ages are reasonably well reproduced by the model, considering the high sensitivity of the results to the applied boundary conditions and the large local variability of flow rates and flow direction. The pneumatic data responding to barometric pressure changes have been simulated, taking into account the effect of the ESF. The simulations results agree very well with the data observed in borehole SD-7.

The liquid flow pattern is again determined by the variable infiltration rates. The modeled flow field is predominantly vertical, with lateral diversions at contacts and due to variations in saturation and water potential. Note, however, that three-dimensional effects may be significant. Furthermore, prediction of transport in the liquid phase requires much higher resolution, especially near sloping layers of low vertical permeability, where water is accumulated and horizontally diverted in a thin layer of relatively high velocity.

Finally, a transient simulation of a high infiltration event demonstrates that small amounts of liquid and potential tracers may travel very fast through the mountain along faults and fractures, explaining the potential of detecting bomb-pulse ^{36}Cl concentration in the Topopah Spring unit.

The simulations discussed here were based on existing parameter sets, i.e. no new data was derived as a result of this modeling study.

12.7 References

- Ahlers, C. F., C. Shan, C. Haukwa, A. J. B. Cohen, G. S. Bodvarsson, Calibration and prediction of pneumatic response at Yucca Mountain, Nevada, using the LBNL/USGS three-dimensional, site-scale model of the unsaturated zone, Yucca Mountain Project Milestone OB12M, Lawrence Berkeley National Laboratory, Berkeley, CA, 1996.
- Fabryka-Martin, J. T., P. R. Dixon, S. Levy, B. Liu, H. J. Turin, and A. V. Wolfsberg, Summary report of Chlorine-36 studies: Systematic sampling for Chlorine-36 in the Exploratory Studies facility, Level 4 Milestone Report 3783AD, Los Alamos National Laboratory, Los Alamos, NM, 1996.
- Loskot, C.L., Geohydrologic Data From Test Hole USW UZ-6s, Yucca Mountain, Nye County, Nevada, Open-File Report 93-60, U.S. Geological Survey, Denver, Colorado, 1993.
ACCN:NNA.19930518.0073
DTN:GS921208312211.013 Non-Q
- Phillips, O. M., Infiltration of a liquid finger down a fracture into superheated rock, *Water. Resour. Res.*, 32, 1665-1670, 1996.
- Patterson, G. L., Data transmittal of pneumatic pressure records from April 4, to June 27, 1996, for borehole USW SD-7, Yucca Mountain, Nevada, U.S. Geological Survey, Denver, Colorado, 1996.
- Pruess, K., TOUGH2 - A general-purpose numerical Simulator for Multiphase fluid and heat flow, Report LBL-29400 UC-251, Lawrence Berkeley National Laboratory, Berkeley, CA, 1991.
ACCN:NNA.19940202.0088
- Pruess, K., and T. N. Narasimhan, On fluid reserves and the production of superheated steam from fractured vapor-dominated geothermal reservoirs, *J. Geophys. Res.*, 87, (B11), 9329-9339, 1982.
ACCN: NNA.19900702.0038
- Pruess, K., and T. N. Narasimhan, A practical method for modeling fluid and heat flow in fractured porous media, *Soc. Pet. Eng. J.*, 25(1), 14-26, 1985.
ACCN: NNA.19890522.0235
- Pruess, K., and Y. W. Tsang, Thermal modeling for a potential high-level nuclear waste repository at Yucca Mountain, Nevada, Lawrence Berkeley National Laboratory Report LBL-35381 UC-600, Lawrence Berkeley National Laboratory, Berkeley, CA, 1994.
ACCN: HQO.19940506.0005
- Pruess, K., A. Simmons, Y. S. Wu, and G. Mordis, TOUGH2 software qualification, Lawrence Berkeley National Laboratory Report LBL-38383 UC-814, Lawrence Berkeley National Laboratory, Berkeley, CA, 1996.

Simulation of Coupled Processes in a Two-Dimensional West-East Cross-Section of Yucca Mountain, Nevada

Rousseau, J. P., C. L. Loskot, J. Kume, M. Kurzmarck, N. D. Brian, K. Thomas, and A. J. Greengard, In-situ borehole instrumentation and monitoring data for USW NRG-7a and USW NRG-6, Yucca Mountain, Nye County, Nevada, 1995.

DTN:GS950208312232.003 Q

Rousseau, J. P., E. M. Kwicklis, and C. Gillies, Eds., Hydrogeology of the unsaturated zone, north ramp area of the Exploratory Studies Facility, Yucca Mountain, Nevada, USGS WRI-96xxxx, U.S. Geological Survey, Denver, Colorado 1996 (draft.)

Thorstenson, D. C., H. Haas, E. P. Weeks, and J. C. Woodward, Physical and chemical characteristics of topographically affected airflow in an open borehole at Yucca Mountain, Nevada, Proceedings of the Topical Meeting on Nuclear Waste Isolation in the Unsaturated Zone FOCUS '89, Las Vegas, NV, 256-270, September 17-21, 1989, American Nuclear Society, 1990.

ACCN:NNA.19900723.0196

DTN: GS930508312261.004 Non-Q

Weeks, E. P., Effect of topography on gas flow in unsaturated fractured rock: concepts and observations, Geophysical Monograph 42, AGU, 165-170, 1987.

ACCN: HQS.19880517.3214

Weeks, E. P., Does the wind blow through Yucca Mountain?, Proceedings of Workshop V: Flow and Transport through Unsaturated Fractured Rock - Related to High-Level Radioactive Waste Disposal, NRC, 43-53, 1991.

ACCN:MOL.19941006.0033

DTN: GS940608312261.003 Non-Q

Wittwer, C., G. Chen, G. S. Bodvarsson, M. Chornack, A. Flint, L. Flint, E. Kwicklis, and R. Spengler, Preliminary development of the LBL/USGS three-dimensional site-scale model of Yucca Mountain, Nevada, Report LBL-37356, UC-814, Lawrence Berkeley National Laboratory, Berkeley, CA, 1995.

Wu, Y. S., G. Chen, and G. Bodvarsson, Preliminary analysis of effects of thermal loading on gas and heat flow within the framework of the LBNL/USGS site-scale model, Report LBL-37729 UC-814, Lawrence Berkeley National Laboratory, Berkeley, CA, December 1995.

Wu, Y. S., S. Finsterle, P. Frazer, and A. Simmons, Software qualification for ITOUGH2 and various equation-of-state (EOS) modules and auxiliary modules for TOUGH2 and ITOUGH2, Report Lawrence Berkeley National Laboratory, Berkeley, CA, August 1996 (draft).

Simulation of Coupled Processes in a Two-Dimensional West-East Cross-Section of Yucca Mountain, Nevada

Yang, I. C., H. H. Haas, E. P. Weeks, and D. C. Thorstenson, Analysis of gaseous-phase stable and radioactive isotopes in the unsaturated zone, Yucca Mountain, Nevada, Proceedings of the NWWA Conference on Characterization and Monitoring of the Vadose (Unsaturated) Zone, 488-506, 1985.
ACCN:NNA.19900403.0266
DTN: GS930508312271.021 Non-Q

THERMAL LOADING STUDIES USING THE UNSATURATED ZONE MODEL

C. Haukwa, Y.S. Wu, and G.S. Bodvarsson

August 1996

13.1 Introduction

13.1.1 Importance of the Thermal Loading Studies

In addition to effects of natural geothermal heat flow, the heat generated as a result of nuclear waste emplacement within the repository will significantly affect fluid flow and heat transfer in the unsaturated zone and the saturated zone immediately below it. Quantitative evaluation of the thermohydrologic effects of thermal loading on the performance of the potential nuclear waste repository at Yucca Mountain is essential for characterization of the behavior of the unsaturated zone and site performance studies, as well as for adequate design of the engineering barrier at the repository.

Extensive studies of the effects of unsaturated zone thermal loading have been carried out (Busheck 1991, 1992, 1993; Duffner, 1993; Nitao, 1988; Pruess, 1990; and Ryder, 1990). All these studies predict extensive boiling due to thermal loading at the repository horizon dependent of the thermal load. The studies, however, do not explicitly include the geology nor do they use simplified horizontal layering along a cross-section.

In this chapter we examine the effects of thermal loading at the repository horizon using a 2-D vertical North-South cross-section (of the 3-D site-scale model), which crosses the entire repository block through its center, and extends about 500 meters below the water table. The model explicitly includes the (UZ-SZ) geological layering along the cross-section. Using this model, we investigate fluid and heat transfer in the unsaturated zone (UZ) and the long term response of the UZ and saturated zone (SZ) to thermal loading at the repository. The numerical simulations reported were carried out using the Q code TOUGH2 (Pruess, 1991).

13.1.2 Thermal Loading and the UZ Model

The effects of thermal loading on the ambient moisture and heat flow were studied using a North - South 2-D vertical cross-section model through the repository block area. Figure 13.1.1 shows the location of the 2-D cross-section A-A' used in this study. This cross-section through the repository block was chosen primarily because it crosses the longest extent of the repository. This section also allows us to investigate the influence of the N-S hydrogeologic layering and the vitric-zeolitic interface in the Calico Hills on fluid flow both at ambient condition and during thermal loading at the repository.

13.1.3 Thermal Goals

Thermal goals (temperature limits) for the rock units within and below the potential repository at Yucca mountain have been documented. (TRW, 1996). One of the temperature limits sets a maximum of 115°C for the interface of the Topopah Springs (TSw) tuff and the underlying Calico Hills (CHn) Non-welded units. This temperature limit was intended to address the concerns that mineralogical changes would occur due to dehydration or re-crystallization induced by repository heating. These changes could have physical and chemical consequences that could be detrimental to waste isolation (TRW, 1996). More recent studies indicate a thermal limit of 90-100°C is more appropriate for the zeolitic Calico Hills units, which are estimated to be about 100 m below the potential repository horizon (TRW, 1996). Another limit sets a maximum of 200°C at one meter distance from the repository drift wall, because silica phase inversion and temperature gradients can adversely affect the thermal mechanical stability of the repository walls. The thermal cladding limit of 350°C was set to address the potential for canister deterioration under thermal loading due to a combination of stress, corrosion and fatigue. Both the repository drift and the waste canisters are on a much smaller spatial scale than that addressed by the 3-D site-scale unsaturated zone model which is intended to provide mountain scale response to thermal loading. Therefore the site scale model will only be used to investigate the potential for violation of only the first thermal limit, i.e. 90-100°C, within the top Calico Hills zeolitic layers.

13.1.4 Purpose of this Study

The purpose of this study is to investigate the effect of repository thermal loading on the temperature distribution and fluid flow paths within the saturated and unsaturated zone. The adequacy of the unsaturated zone model and the ECM scheme in prediction of the evolution of temperature within the unsaturated zone will be explored. We further investigate the need for using a combined saturated-unsaturated zone model in simulating the UZ thermal response.

13.1.5 Modeling Approach

In this study the repository is represented by a 6.0 m thick zone which is over 4 km along the cross section with an average elevation of 1,070 masl. The repository horizon is modeled with a slope of a gradient of about 1% in order to maintain the repository at a minimum 50 m above the Calico Hills unit. This results in a nearly 40 m difference in elevation over the 4 km repository length. This is consistent with the 3-D model and it is designed to accommodate the dipping in the geological layering in the north, south and west boundaries of the repository domain (Chapter 5, this report). For thermal loading studies we assume that thermal loading at the repository horizon over the emplacement period can be represented by an equivalent uniform thermal load at an Area Power Density (APD) of 83 kW/acre. At this thermal load, equivalent generic total heat versus time decay curves (M&O, 1995) were used to provide a time dependent heat generation table. This provides a transient heat source at the repository. Under this thermal loading scenario, we performed numerical simulations for the following cases: 1) Net infiltration rate of 0.1 mm/year

using the ECM method; 2) Infiltration rate of 4.4 mm/year, using the ECM model; 3) Infiltration rate of 4.4 mm/year using a dual-permeability (dual-k) model. The simulations were carried out for a maximum time of 100,000 years to investigate both the heating and cool down cycles after waste emplacement.

13.1.5.1 Numerical Grid, Material Properties and Boundary Conditions for UZ Thermal Loading Studies

Figure 13.1.1 shows a plan view of the 3-D-model and the location of the N-S 2-D vertical cross-section (A-A') used in the thermal hydrological studies. The 2-D vertical cross-section used in this study is refined from the 3D site scale model and has a total of 3774 elements and 6438 connections. For thermal studies this 2-D vertical cross-sections extends 500 below the water table into the saturated zone, down to the Tram Tuff hydrogeological model unit. This extension allows for explicit coupling of the saturated and the unsaturated zone in order to examine the effects of thermal loading on the water table and the saturated zone.

Figure 13.1.1
Areal grid of the 3-D UZ model showing location of N-S cross-section, boreholes.

The repository horizon is explicitly represented by a 6 m thick repository layer, bounded by 10 m thick layers. This repository horizon is mainly within the Topopah Springs model stratigraphic sub-layer five. The final model con-

sists of 27 non-uniform grid layers in the four welded and non-welded hydrogeological units (Chapter 2, this report).

The material properties of rocks are explicitly allocated based on the elevation of element node, model layer and the hydrogeological unit thickness. The pinchout of the Paintbrush, (PTn-2 and PTn-4) sub-layers as well as the zeolitic-vitric interface in the top of the Calico Hills (CHn) unit is explicitly modeled. Rock properties required for numerical simulations in the Tiva Canyon (TCw), Paintbrush (PTn), Topopah Springs (TSw), and Calico Hills (CHn) units were obtained from inverse modeling studies using moisture tension and liquid saturation data (Bandurraga et al., 1996, Chapter 3, this report). Different material properties were obtained depending on the infiltration rate assumed in the inversions in Chapter 3. For the thermal loading studies we use properties obtained for a uniform infiltration rate of 0.1 and spatially variable rates averaging 4.4 mm/year. The properties for the vitric and zeolitic Bullfrog (Bf) units as well as the Tram (TM) vitric and zeolitic units below the water table were assumed to be the same as for the Prow Pass model layers, since there are not sufficient data available to do an inversion for the saturated zone in the 3D site scale model.

Figure 13.1.2

2-D UZ North-South Cross section A-A', showing model grid layers and hydrogeological units used.

The model parameters for the 2-D cross-sections were the same as those for the 3-D model unsaturated flow studies (Chapter 8, this report). For the thermal studies the following additional thermal properties and model boundary conditions were used.

Constant temperature and constant pressure conditions are specified on both top and bottom boundaries. The bottom boundary temperature was based on the observed temperature distribution from bore holes and the geothermal heat-flow maps (Bodvarsson et al., 1996, Chapter 9, this report). The top boundary temperature was calculated based on surface elevation and observed mean annual temperature. The spatially variable bottom boundary temperature, at 500 m below the water table, is based on extrapolation of temperature profiles and using estimated saturated thermal conductivity of these formations. This extrapolation results in an increase of about 5°C from the measured values at the water table. The thermal conductivities used in the model are based on estimated saturated and unsaturated thermal conductivity of the hydrogeologic units (Sass et al., 1988). Steady state saturated zone conditions were computed assuming a water table at 730 masl, and a hydrostatic gradient below the water table. Other properties used in the model have already been discussed Chapters 3 and 4.

Boreholes UZ-14, G-1, G-2, H-3, H-5 and UZ-6 are within 300 m of this cross-section were used to control geological layering (Figure 13.1.2). Borehole UZ-14 was in addition used to validate the rock properties using the observed saturation data (Figure 13.1.3). Our computed ambient liquid saturations matches well with the measured saturation data in UZ-14, as shown in Figure 13.1.3.

Figure 13.1.3

Comparisons between the observed and simulated saturation for borehole UZ-14, using the 2-D section, the USGS measured values, and infiltration rate of 0.1 mm/year. Data from L. Flint, USGS.

**13.1.5.2
ECM and Dual-k Approaches**

The saturated zone and the unsaturated zone at Yucca Mountain consist of different hydrogeologic units that exhibit varying degrees of fracturing. The Tiva Canyon (Tcw), and the Topopah Springs (TSw) hydrogeologic units contain extensive vertical conductive fractures. The Paintbrush (PTn), and vitric CHn though very permeable, shows little evidence of fracturing. The zeolitic Calico Hills hydrogeologic units have a low permeability matrix with few fractures (Chapter 3, this report).

Numerical models of geological systems generally consist of large computational blocks. For example, the 3-D Site Scale model consists of grid blocks with an average dimension of 10-100 m. These large blocks contain tens to hundreds of fractures that are combined with the matrix to provide an effective continuum with hydraulic properties that mimic the behavior of both the matrix and the fractures. This method of modeling fractured porous media is called the ECM (Effective Continuum method, Chapter 4, this report).

In order to effectively capture the physics of the response of a fractured porous medium and to evaluate the effectiveness of the ECM approach, we also developed a dual-permeability model for the new 3-D model (Wu et al., Chapter 8, 1996) and the 2-D cross-section model of the Yucca mountain.

For the dual-k model a fracture porosity of 1% was used with fracture aperture and density the same as those used in the 3-D model (Chapter 8, this report). The PTn and the saturated zone were simulated using the ECM. The dual-k model was used to simulate thermal loading using an infiltration of 4.4 mm/year (Flint, 1996), which is the average of the spatially variable rates.

**13.2 *ECM simulation Results with 0.1 mm/year
Infiltration***

**13.2.1
Temperatures**

Figure 13.2.1 shows the ambient temperature in the 2-D cross-section using a uniform infiltration of 0.1 mm/year and the ECM model. The temperature is mainly controlled by the geothermal gradient and the saturated thermal conductivity (Data from Sass et al., 1988). This ambient temperature distribution is consistent with inferred heat flow maps and the temperature distribution at the water table (Chapter 9, this report). Estimated ambient temperatures at the repository horizon is 23-26°C and about 29-32°C at the water table.

Starting with these ambient conditions, as shown in Figure 13.2.1, a time dependent heat source was applied uniformly at the repository horizon for a total of 100,000 years. The heat source was based on tabulated heat decay data at an equivalent APD of 83 kW/acre (M&O, 1995). Figures (13.2.1- 13.2.6) show the evolution in temperature for this case. Boiling begins 10 years after thermal loading is imposed. For a period of 10-2000 years following emplace-

ment, a complete dry-out zone develops at the repository. The peak temperature rises to 104° C at the central part of the repository. In the regions immediately above and below the repository, boiling also occurs. Within the central part of the potential repository, this boiling zone extends about 100 meters above and below the dry-out region, as shown in Figures. 13.2.2 and 13.2.4. In this zone convective heat transfer dominates with the temperature at about 97°C.

In 1,000 years the temperature above the central heated area of the 2-D cross-section rises substantially. The temperature increases to about 10°C at the ground surface, the temperature rises to 55°C at 50 m below the water table (Figure 13.2.3). At this time the repository temperature is 104°C, the temperature at the base of the PTn is 67°C and the temperature at the top of the Calico Hills is 92°C. The computed maximum temperature at the water table is 59°C in about 5,000 years, long after repository temperatures have decreased (Figure 13.2.3, 13.2.4).

At the repository horizon temperatures rise to boiling conditions within 10-100 years and remain constant (Figure 13.2.5). After 2,000 years the computed unsaturated zone and repository temperatures begin to decline, although local boiling still occurs at the repository horizon. In 10,000 years the repository temperature drops to 70°C and is 30°C after 100,000 years. The computed near-surface temperature (Figure 13.2.6) shows local variation along the cross-section, dependent mainly on the elevation of the surface. Peak temperature is 29°C, which is about 12°C above the ambient value, and occurs after 500-1,000 years of thermal loading.

Figure 13.2.1 2-D UZ cross-section model. Ambient temperature at infiltration rate 0.1 mm/year.

Figure 13.2.2

Temperature distribution after 1000 years thermal loading. APD = 83 kW/acre, infiltration = 0.1 mm/year.

r.

Figure 13.2.3

Vertical temperature profiles through the center of the repository block during 1,000 years of thermal loading. APD = 83 kW/acre, infiltration = 0.1 mm year.

Figure 13.2.4

Temperature at various depths at the center of the repository during 100,000 years of thermal loading. APD = 83 kW/acre, infiltration = 0.1 mm/year.

Figure 13.2.5

Temperature in the repository horizon during thermal loading, APD 83 kW/acre, infiltration = 0.1 mm/year.

Figure 13.2.6

Temperature at the land surface during thermal loading, APD 83 kW/acre, infiltration = 0.1 mm/year.

13.2.2 Saturation

Figure 13.2.7 to 13.2.11 show the variation of saturation in the matrix and fracture continua in the 2-D cross-section at a uniform infiltration of 0.1 mm/year. Under ambient conditions, (Figure 13.2.7), most of liquid phase in the unsaturated zone remains in the matrix continuum with a high liquid saturation in the zeolitic Calico units. As discussed before, the simulated ambient saturation matches the measured data for UZ-14 (Figure 13.1.3). The fracture continuum shows low liquid saturation, particularly in the bottom layers of the TSw and vitric Calico Hills, Prow Pass and Bullfrog layers. Thermal loading causes substantial changes in the saturation distribution, especially near the repository region. For this case we examine the evolution of saturation in the matrix and fracture continua to understand the behavior of the unsaturated zone moisture flow under thermal loading. Boiling conditions exist at the repository and the regions immediately above and below the repository. Throughout the thermal loading cycle the boiling zone is confined to the upper layers of the TSw, and it does not extend into the PTn (Figure 13.2.8-13.2.9). During the boiling period, the saturations inside and outside the boiling zone show both spatial and temporal variations, which are produced by a complex evolution of boiling and condensation processes over time.

In about 500 years the liquid saturation at the repository horizon drops to zero and matrix liquid saturation at the top of the Calico Hills rises slightly due to vapor condensation, as shown in Figure 13.2.9. Figure 13.2.10 shows the evolution of saturation in a vertical column of the center of the repository. Repository thermal loading leads to a localized decrease in matrix saturation in the regions above and below the repository. Two condensation caps are formed

near the southern and northern ends of the repository, where rapid cooling by convection cells maintains low local temperatures (Figure 13.2.12).

Until 2,000 years the repository region remains relatively dry as repository as the rate of vaporization exceeds the net infiltration. The gas flux vectors show strong convection patterns near the repository. Circulation cells develop near both ends of the repository, and gas flows away from the repository in the central region above and below the repository horizon. Below the repository the condensate flows laterally along the zeolitic-vitric interface into the vitric zones, because of the low permeability in the zeolitic formations. The lowest saturation at the repository occurs in the period when the largest boiling zone developed (Figure 13.2.11).

Figure 13.2.7
Ambient liquid saturation in the matrix and liquid flux, infiltration = 0.1 mm/year.

Figure 13.2.8

Liquid Saturation after 1000 years thermal loading APD = 83 kW/acre, infiltration = 0.1 mm/year.

Figure 13.2.9

Liquid saturation at various depths in the center of the repository block during 100,000 years of thermal loading. APD = 83 kW/acre, infiltration = 0.1 mm/year.

Figure 13.2.10
Vertical saturation profiles through the center of the repository block during 100,000 years of thermal loading. APD = 83 kW/acre, infiltration = 0.1 mm/year.

Figure 13.2.11
Liquid saturation in the repository horizon during thermal loading, APD 83 kW/acre, infiltration = 0.1 mm/year.

13.2.3 Percolation Flux

Under ambient conditions, the percolation flux at the repository is almost the same as the infiltration rate used in the simulation and the flow is mainly vertical at about 0.1 mm/year (Figure 13.2.7). With thermal loading effects, heat generated by the emplaced waste results in large increases in both gas and

liquid percolation flux around the repository, due to vaporization, pressurization, desaturation, and strong capillary suction.

For most of the simulated thermal loading period the repository acts as a barrier to downward water movement. Some lateral flow develops at a zone of 100 - 150 m above the repository, mainly within the TSW due to strong gas convection and vapor condensation (Figure 13.2.12). Above the boiling zone, temperature drops rapidly, and vapor mixes with downward flowing infiltrated water, which results in vapor condensation. Below the repository, liquid is displaced by expanding gases down to the zeolitic Calico Hills layers which causes southward lateral flow. At the zeolitic/vitric interface, a zone with high liquid vertical flux develops and extends down to the water table (Figure 13.2.12). The source of this the liquid is vapor condensation.

Figures 13.2.13 and 13.2.14 show respectively the vertical liquid fluxes on the top and bottom boundaries of the 6 m repository. On the figures, "positive" flux values denote downward flow, and "negative" denote upward flow. As shown in the two figures, the liquid flux has increased by 3-4 orders of magnitude compared to the ambient flux during 10-500 years after waste emplacement (prior to total dry-out). There is also enhanced liquid flow towards the repository horizon from above and below. At bottom of the repository, strong capillary suction overcomes gravity. Throughout the thermal loading cycle liquid flow at repository horizon is always towards the repository.

Figure 13.2.12

Gas flux profiles in the repository horizon after 1000 years emplacement, APD= 83 kW/acre, infiltration = 0.1 mm/year.

Figure 13.2.13

Liquid Flux crossing the top boundary of the repository, APD = 83 kW/acre, Infiltration 0.1 mm/year.

Figure 13.2.14

Liquid Flux crossing the bottom boundary of the repository, APD = 83 kW/acre, Infiltration 0.1 mm/year.

13.3 *ECM Simulation Results with 4.4 mm/year Infiltration*

13.3.1 Temperature

The ambient temperature distribution simulated using the ECM model with a uniform infiltration rate of 4.4 mm mm/year is almost the same as the one obtained using a 0.1 mm/year infiltration rate (Figure 13.2.1). This indicates that the temperature is mainly controlled the by fixed geothermal gradient and the thermal conductivity, and is not significantly affected by the infiltration rates used. Starting with these ambient conditions, a time dependent heat source was applied uniformly at the repository horizon for a total of 10,000 years, as in the previous case.

Figures 13.3.1- 13.3.6 show the evolution of temperature for this case. As for the 0.1 mm/year infiltration case, boiling conditions develop in 10 years. After 100 years (Figure 13.3.1-13.3.3), a boiling zone, extends about 50 m above and below the repository. This boiling condition continues for 2000 years of thermal loading. Unlike the case for 0.1 mm/year infiltration, complete dry-out conditions do not develop at the repository throughout the thermal loading cycle, because net liquid influx exceeds the rate of vaporization at the repository horizon. Within the central part of the potential repository, the boiling zone extends further, reaching a maximum of 50 m below and 150 m above the repository horizon during 500 to 1,000 years the (Figures. 13.3.1-13.3.3). In the boiling zone convective heat transfer dominates, and the temperature remains constant at about 95°C. In 1,000 years, the temperature at the land surface above the central heated area of the 2-D cross-section rises to 28°C, and to 93°C at the base of the PTn. The temperature is 95°C at the repository, 75°C at the top of Calico Hills and 55°C 50 m below the water table (Figure 13.3.4). The computed maximum temperature at the water table is 58°C and occurs in 5,000 years, long after repository temperatures have decreased (13.3.3, 13.3.4).

At the repository horizon temperatures rise to boiling conditions from 10 to 100 years and remain constant for several thousands of years thereafter (Figure 13.3.5). After 2,000 years the computed unsaturated zone and repository temperatures begin to decline even though local boiling still persists at the repository horizon. In 10,000 years, maximum temperature is only 72°C at the repository. The computed surface temperature (Figure 13.3.6) shows local variations dependent mainly on the elevation of the ground surface. Maximum temperature at the land surface is 31°C, or 14°C above the ambient condition, after 500-1000 years of thermal loading

Although computed maximum temperature at the repository horizon is less than that for the 0.1mm case, the temperatures above the repository horizon are higher since, in this case, the boiling zone is mainly above the repository horizon.

Figure 13.3.1

Temperature distribution after 1000 years thermal loading. ECM, APD = 83 kW/acre, infiltration = 4.4 mm/year. Vectors and flow paths show liquid Flux in matrix continuum.

Figure 13.3.2

Temperature distribution after 1000 years thermal loading. ECM; APD = 83 kW/acre, infiltration = 4.4 mm/year. Vectors and flow paths show Gas flux matrix continuum.

Figure 13.3.3
Vertical temperature profiles through the center of the repository block during 10,000 years of thermal loading; ECM, APD = 83 kW/acre, infiltration = 4.4 mm/year.

Figure 13.3.4
Temperature at various depths at the center of the repository during 10,000 years of thermal loading; ECM, APD = 83 kW/acre, infiltration = 4.4 mm/year.

Figure 13.3.5
Temperature in the repository horizon during thermal loading; ECM, APD 83 kW/acre, infiltration = 4.4 mm/year.

Figure 13.3.6
Temperature at the land surface during thermal loading; ECM, APD 83 kW/acre, infiltration = 4.4 mm/year.

**13.3.2
Saturation**

Figures 13.3.7 and 13.3.8 show the ambient saturation in the matrix and fracture continua in the 2-D cross-section. Most of the liquid phase in the unsaturated zone is in the matrix continuum (Figure 13.3.8). The fracture continuum has low saturation, particularly in the bottom layers of the TSw and vitric Calico Hills, Prow Pass and Bullfrog layers. Thermal loading significantly changes the saturation distribution, particularly, near the repository region. For this case we examine the evolution of saturation in the matrix and fracture continua to understand the behavior and effects of thermal loading on moisture flow and distribution in the unsaturated zone. In particular we are interested in short and long term responses, to be compared with dual-k modeling results.

As discussed before, the extent of the boiling zone, as indicated by the temperature profiles, is up to 150 m above and 50 m below the repository horizon. This boiling zone extends to the base of the PTn units in 100-1000 years. During the thermal loading cycle, the saturation distributions are significantly changed, spatially and temporally, near the repository boiling zone in the unsaturated zone. Figure 13.3.9 and 13.3.10 show the saturation in the matrix and fracture continuum at 1,000 years. Repository thermal loading leads to a decrease in saturation of the matrix close to the repository and an increase in saturation in the condensation zone, at 50 m above the repository (Figure 13.3.9). During this period the net influx into the repository exceeds the rate of vaporization caused by heating. Under the high infiltration rate, there is a net downward flow, even through the low permeability zeolitic Calico Hills Formations, throughout the thermal loading cycle. The gas flux vectors also show strong convection patterns near the repository.

To better understand the evolution of saturation and evaluate the rewetting phase in the thermal loading cycle we examined a 1-D vertical column at the center of the repository. For this column the evolution of saturation in the matrix continuum over the loading cycle was investigated (Figures 13.3.11, 13.3.12). The saturation in the matrix is found to change significantly only in the boiling zone, within 100 m from the repository. The minimum saturation is 0.38 for the matrix continuum, in about 100 years, when boiling conditions are established. Between 100 and 1000 years, boiling continues and expands, but the liquid saturation within the boiling zone rises. In this zone convective heat transfer dominates with a constant temperature at about 95°C. After 100 years, the rate of heat generation from the repository is not high enough to vaporize the liquid influx into the boiling region, causing the liquid saturation to increase.

Matrix liquid saturation at the top of the CHn increases and reaches its maximum in 100 years (Figure 13.3.11). The increase in saturation at the top of the CHn is mainly due to condensation of repository heat driven vapor flux. Figure 13.3.12 shows that maximum saturation changes in saturation are within about 100 m of the repository horizon. The matrix saturation at the southern and northern ends of the repository remains essentially unchanged

throughout the thermal loading cycle (Figure 13.3.13) and that rewetting of the repository horizon occurs uniformly. At about 1,000 years, though the boiling zone is still extensive, the average matrix liquid saturation at the repository recovers to a value of 0.85 from about 0.38 at 100 years. Rewetting of the de-saturated zone leads to an end of the boiling period and the decline in saturated zone temperature.

Figure 13.3.7

Matrix continuum ambient liquid saturation; ECM, APD 83 kW/acre, infiltration = 4.4 mm/year. Vectors show liquid flux in matrix.

Figure 13.3.8

Fracture continuum ambient liquid saturation; vectors show liquid flux; ECM, APD 83 kW/acre, infiltration = 4.4 mm/year. Vectors show liquid flux in fractures.

Figure 13.3.9

Matrix continuum liquid saturation after 1000 years thermal loading, APD = 83 kW/acre, infiltration = 4.4 mm/year; ECM.

Figure 13.3.10

Fracture continuum liquid saturation after 1000 years thermal loading ECM, APD = 83 kW/acre, infiltration = 4.4 mm/year; vectors show liquid flux.

Figure 13.3.11

Liquid saturation at various depths in the center of the repository block during 10,000 years of thermal loading; ECM, APD = 83 kW/acre, infiltration = 4.4 mm/year.

Figure 13.3.12

Vertical saturation profiles through the center of the repository block during 10,000 years of thermal loading; ECM, APD = 83 kW/acre, infiltration = 4.4 mm/year.

Figure 13.3.13

Liquid saturation in the repository horizon during thermal loading; ECM, APD 83 kW/acre, infiltration = 4.4 mm/year.

13.3.3 Percolation Flux

The changes in percolation flux at the repository horizon are associated closely with changes in saturation conditions, which are related to the intensity of boiling, dry-out and rewetting processes. Figure 13.3.14-13.3.15 show the detailed evolution of the vertical liquid fluxes versus thermal loading time on the top and bottom boundaries of the repository. Similar to the case of the lower infiltration of 0.1 mm/year, Figure 13.3.14 and 13.3.15 show a huge increase in the liquid flux into the repository during the thermal loading, and no liquid flow out.

For the first 10 years after waste emplacement, repository liquid saturation decreases and the liquid influx into the repository increases by a factor of 10 to 30 due to strong capillary suction, as compared with the ground surface infiltration (Figure 13.3.14). This indicates that most of the influx liquid is released from the nearby matrix or condensation, not from the surface infiltration. After 100 years the influx into the repository decreases to an average of about 10 mm/year at the bottom boundary and about 60 mm/year at the top boundary of the repository.

Figure 13.3.14
Liquid Flux crossing the top boundary of the repository; ECM, APD = 83 kW/acre, Infiltration 4.4 mm/year.

Figure 13.3.15
Liquid Flux crossing the bottom boundary of the repository; ECM, APD = 83 kW/acre, Infiltration 4.4 mm/year

13.4 Dual-k Simulation Results with 4.4 mm/year Infiltration

13.4.1 Temperature

The ambient temperature in the 2-D cross-section, simulated using the dual-k model with an infiltration rate of 4.4 mm/year, is similar to that of the ECM case. As in the ECM study, the dual-k simulation uses the thermal loading scenario of an equivalent APD of 83 kW/acre. Figure 13.4.1 to 13.4.8 show the spatial and temporal changes in temperature for this case. Boiling conditions develop after about 100 years of thermal loading. At 500 years (Figure 13.4.1, 13.4.2), the temperatures within the zone 100 m above and below the repository reach 95°C, and strong convective heat transfer occurs at or near boiling conditions. This boiling condition lasts for an additional 500 years (Figure 13.4.3 and 13.4.4). Unlike in the case of the ECM study with 4.4 mm/year infiltration, complete dry-out conditions do not develop at the repository throughout the thermal loading cycle.

The simulated boiling zone extends to a maximum of 100 m vertically above and below the repository horizon for 500-1000 years, as shown in Figure 13.4.5. In this period, convective heat transfer dominates and the temperature remains constant at about 95°C in the boiling zone. In 1,000 years, temperature near the land surface rises to about 25°C, and 65°C at the base of the PTn. At the same time, the repository temperature reaches 94°C, and the temperatures at the top of Calico Hills and at 50 m below the water table are at 76°C and 57°C (Figure 13.4.6), respectively. The computed maximum temperature at the water table is 59°C, which occurs at about 5,000 years.

At the repository horizon temperatures rise to boiling conditions in 20-100 years and remain constant (Figure 13.4.5, 13.4.6 and 13.4.7) until 2,000 years when the computed repository temperatures begin to gradually decline. After 10,000 years temperature at the repository, decreases to 60°C, and further drops to 42°C after 25,000 years. The computed surface temperature (Figure 13.4.8) shows that the highest temperature near the ground surface is 28°C in 1,000 years.

Predicted temperature at the surface and at the base of the PTn are less than those obtained from the ECM case at the same infiltration rate, since, in this case, boiling extends further below the repository. However, both the Dual-K and ECM predict similar temperature rise at the top of the Calico Hills (75-76°C) which are well below the breakdown temperature for zeolites.

Figure 13.4.1

Temperature distribution after 500 years thermal loading; Dual-k, APD = 83 kW/acre, infiltration = 4.4 mm/year. Vectors and flow paths show liquid flux in matrix continuum.

Figure 13.4.2

Temperature distribution after 500 years thermal loading; Dual-k, APD = 83 kW/acre, infiltration = 4.4 mm/year. Vectors and flow paths show liquid flux in fracture continuum.

Fig 13.4.3
Temperature distribution after 1000 years thermal loading; Dual-k, APD = 83 kW/acre, infiltration = 4.4 mm/year. Vectors and flow paths show gas flux in matrix continuum.

Figure 13.4.4
Temperature distribution after 1000 years thermal loading; Dual-k, APD = 83 kW/acre, infiltration = 4.4 mm/year. Vectors and flow paths show liquid flux in matrix continuum.

Figure 13.4.5

Vertical temperature profiles through the center of the repository block during 25,000 years of thermal loading; Dual-k, APD = 83 kW/acre, infiltration = 4.4 mm/year.

Figure 13.4.6

Temperature at various depths at the center of the repository during 25,000 years of thermal loading; Dual-k, APD = 83 kW/acre, infiltration = 4.4 mm/year.

Figure 13.4.7

Temperature in the repository horizon during thermal loading; Dual-k, APD 83 kW/acre, infiltration = 4.4 mm/year.

Figure 13.4.8

Temperature at the land surface during thermal loading; Dual-k, APD 83 kW/acre, infiltration = 4.4 mm/year.

13.4.2 Saturation

Figures 13.4.9 and 13.4.10 show the simulated ambient saturations, for the matrix and fractures, respectively. As can be seen from the figures, the liquid saturations in the matrix are much higher than those in the fractures. These ambient saturation distribution in the fracture and matrix continua is very similar to the ambient saturation for the ECM case with 4.4 mm/year infiltration.

Figure 13.4.11 and 13.4.12 show the matrix saturation distributions after 500 and 1000 years of thermal loading, respectively. The matrix saturation at the repository is the lowest in 500 years. After 500 years the matrix saturation at the repository horizon increases, while temperature remains nearly constant during this period (Figure 13.4.5). As in the ECM case, not enough heat is generated to vaporize the liquid influx towards the repository.

The gas flux shows strong convection patterns near the repository throughout the boiling period (Figure 13.4.13 and 13.4.14). Circulation cells develop at both the southern and northern ends of the repository. Vapor condensation zones are formed directly above the repository, below the TCw. This condensed liquid drains back to the repository, resulting in a local increase in influx at the top boundary of the repository. Below the repository heat driven gas flow moves up-dip of the repository, along the top of Calico Hills to form circulation cells at the southern end of the repository (Figures 13.4.14).

To better understand the saturation changes and the rewetting processes in the thermal loading cycle, we again use a 1-D vertical column from the 2-D grid to look at saturation variations (Figures 13.3.15a, 13.3.15b) in the matrix and the fracture continua. The matrix saturation changes along the column are shown in Figure 13.4.15a, and the fracture saturations are presented in Figure 13.4.15b. The minimum matrix liquid saturation is about 40%, and the fracture saturation is as low as 5%, at about 100 years, as soon as boiling conditions are established. Like the ECM case with 4.4 mm/year infiltration, no complete dry-out occurs in either the fracture or matrix with the dual-k simulations.

Liquid saturation at the top of the Calico Hills rises slightly in about 100 years, both in the matrix and the fracture continuum (Figures 13.4.16, 13.4.17). This saturation increase is mainly due to condensation of repository driven vapor flux. Figure 13.4.18 shows that matrix saturation near the south and north ends of the repository horizon remains unchanged throughout the thermal loading cycle and that rewetting processes are very uniform. In 1,000 years of thermal loading, though the boiling zone is still extensive, average liquid saturation at the repository recovers to 75% in the matrix (Figure 13.4.18), and to 15% in the fractures (Figure 13.4.19). A comparison of Figure 13.4.18 and 13.4.19 shows that rewetting of the fracture continuum lags significantly behind that for matrix continuum.

Figure 13.4.9

Matrix continuum ambient liquid saturation; Dual-k, APD 83 kW/acre, infiltration = 4.4 mm/year. Vectors show liquid flux in matrix.

Figure 13.4.10

Fracture continuum ambient liquid saturation; vectors show liquid flux; Dual-k, APD 83 kW/acre, infiltration = 4.4 mm/year. Vectors show liquid flux in fractures.

Figure 13.4.11

Matrix continuum liquid saturation after 500 years thermal loading Dual-k, APD = 83 kW/acre, infiltration = 4.4 mm/year.

Figure 13.4.12

Matrix continuum liquid saturation after 1000 years thermal loading Dual-k, APD = 83 kW/acre, infiltration = 4.4 mm/year.

Figure 13.4.13

Fracture continuum liquid saturation after 500 years thermal loading Dual-k, APD = 83 kW/acre, infiltration = 4.4 mm/year.; vectors show liquid flux.

Figure 13.4.14

Fracture continuum liquid saturation after 1000 years thermal loading Dual-k, APD = 83 kW/acre, infiltration = 4.4 mm/year.; vectors show liquid flux.

Figure 13.4.15a

Matrix vertical saturation profiles through the center of the repository block during 25,000 years of thermal loading; Dual-k, APD = 83 kW/acre, infiltration = 0.1 mm/year.

Figure 13.4.15b

Fracture vertical saturation profiles through the center of the repository block during 25,000 years of thermal loading; Dual-k, APD = 83 kW/acre, infiltration = 0.1 mm/year

Figure 13.4.16
Matrix Liquid saturation at various depths in the center of the repository block during 10,000 years of thermal loading; Dual-k, APD = 83 kW/acre, infiltration = 4.4 mm/year.

Figure 13.4.17
Fracture Liquid saturation at various depths in the center of the repository block during 10,000 years of thermal loading; Dual-k, APD = 83 kW/acre, infiltration = 4.4 mm/year.

Figure 13.4.18
Matrix Liquid saturation in the repository horizon during thermal loading; Dual-k, APD 83 kW/acre, infiltration = 4.4 mm/year.

Figure 13.4.19
Fracture Liquid saturation in the repository horizon during thermal loading; Dual-k, APD 83 kW/acre, infiltration = 4.4 mm/year.

13.4.3 Percolation Flux

The repository percolation fluxes simulated by the dual-k model are shown in Figures 13.4.20-13.4.23. Figures 13.4.20 and 13.4.21 gives the liquid influx into the repository from matrix flow Figures 13.4.22 and 13.4.23 show the influx

from the fracture. As can be seen from the four figures, both matrix flow and fracture flow into the repository increase by as much as 10 times, during the thermal loading period compared to the ambient infiltration rate of 4.4 mm/year. It is interesting to note that the contribution of the fracture flow into the repository is no more than 10 to 20% of the total liquid influx. This suggests that the matrix flow is more important to the rewetting processes of the repository during the thermal loading cycle.

Figure 13.4.20
Matrix liquid flux crossing the top boundary of the repository; Dual-k, APD = 83 kW/acre, Infiltration 4.4 mm/year.

Figure 13.4.21
Matrix liquid flux crossing the bottom boundary of the repository; Dual-k, APD = 83 kW/acre, Infiltration 4.4 mm/year.

Figure 13.4.22
Fracture liquid flux crossing the top boundary of the repository; Dual-k, APD = 83 kW/acre, Infiltration 4.4 mm/year.

Figure 13.4.23

Fracture liquid flux crossing the bottom boundary of the repository; Dual-k, APD = 83 kW/acre, Infiltration 4.4 mm/year.

13.5 Comparisons of Percolation Fluxes Using the Two Modeling Approaches.

13.5.1 Liquid Fluxes

The simulated liquid percolation fluxes using the ECM and the dual-k approaches are compared in Figures 13.5.1 and 13.5.2. Figure 13.5.1 shows spatial distributions of the liquid fluxes along the repository at different times. The figure indicates a similar pattern of the flux variations over the thermal loading period. However, Figure 13.5.1 and 13.5.2 show that at an early time, 10 years, the ECM model predicts a much higher downward matrix flow into the repository. At the same time the dual-k model gives much smaller vertical flow, about at the ambient condition. The reason is a much "drier" condition obtained from the ECM model at this time. At later times, after 100 years, the two models give similar flux calculations. The flow crossing the bottom boundary of the repository, is very similar for the two models during the entire thermal loading period.

Fig 13.5.1

Matrix liquid flux crossing the top and bottom boundary of the repository; for different infiltration rates; ECM and Dual-k, APD = 83 kW/acre; the numbers on curves correspond to the following; a) 1-3 is for (10, 50, 100 years), 0.1 mm/yr., bottom boundary; b) 4-6 is for (10, 100, 1000 years), 0.1 mm/yr., top boundary; c) 7-9 is for (10, 100, 1000 years), 4.4 mm/yr., ECM bottom boundary; d) 10-12 is for (10, 100, 1000 years), 4.4 mm/yr., ECM, top boundary; e) 13 is for 100 years 4.4 mm/yr., Dual-k, top boundary, fracture, f) 14-16 is for (100, 500, 1000 years) 4.4 mm/yr., Dual-k, top boundary, matrix.

Figure 13.5.2

Matrix liquid flux crossing the top and bottom boundary at the center of the repository; for different infiltration rates; ECM and Dual-k, APD = 83 kW/acre.

13.5.2 Gas Fluxes

Similar to the comparisons with liquid fluxes, discussed above, Figures 13.5.3 and 13.5.4 shows the simulated gas mass fluxes using the ECM and the dual-k approaches at the repository. As shown in the two figures, similar gas fluxes are predicted by the models. The only notable difference is at early times. During the early times the ECM model predicts much higher gas fluxes than those from the dual-k model. The gas flow is affected significantly by thermal loading near the repository, and increases by many orders of magnitude from 10 to 1,000 years. After 1,000 years, gas flow gradually decreases to ambient conditions.

Figure 13.5.3

Matrix and Fracture gas flux crossing the top and bottom boundary of the repository; for different infiltration rates; ECM and Dual-k, APD = 83 kW/acre

Figure 13.5.4

Matrix and Fracture gas flux crossing the top and bottom boundary at the center of the repository; for different infiltration rates; ECM and Dual-k, APD = 83 kW/acre.

13.6 Concluding Remarks

A systematic study of effect of thermal loading on the moisture, gas and heat flow in the unsaturated zone of Yucca Mountain has been carried out. The study is based on a 2-D north-south vertical cross-section, using both the ECM and the dual-k modeling approaches. The 2-D model covers both unsaturated and saturated zones to investigate the effects of the water table thermal conditions. Numerical simulations were carried out using the Q code TOUGH2, and the Q equation of state model EOS3, but are based on the non-Q geological model and parameters discussed in Chapters 2 and 3. Based on this data model and parameters, we obtain the following conclusions which are overall non-Q but are scientifically valid.

Examination of the temperature profiles during thermal loading indicates that the location of the model bottom boundary at the water table or at 500 meters below the water table does not affect repository thermo-hydrological behavior during the boiling period under thermal loading. However the coupled UZ-SZ model predicts about a 30°C temperature increase at the water table. This indicates that if a fixed temperature boundary is applied at the water table, the model may overestimate the rate of cooling of the repository.

Thermal loading at the repository results in significant changes in the moisture and temperature distributions in the Mountain. Strong liquid and

gas flow fields several orders of magnitude above ambient develop near the repository. With the thermal loading scenario and the coarse grid used, the maximum temperature at the repository is 104°C for 0.1 mm/year infiltration case and about 95°C for the 4.4 mm/year infiltration. The average temperature of the boiling zone is about 95°C . This boiling zone is confined to the TSw hydrogeological unit.

The simulations show that there is substantial increase in near surface temperatures, about $10\text{-}20^{\circ}\text{C}$ in the area directly above the repository. The predicted maximum surface temperature occurs 750-1000 years after thermal loading begins. The predicted maximum temperature for top of the Calico Hills is about 92°C for the 0.1 mm/yr infiltration case, but about $75\text{-}76^{\circ}\text{C}$ for the 4.4 mm/yr infiltration case. Therefore, at low infiltration rates, temperatures on top of the Calico Hills could lead to mineral changes in the Zeolitic units.

The intensity of the boiling and rewetting processes at the repository are controlled by the available heat and liquid at the repository horizon. For the low infiltration rate case, the repository "dries out" after 100 to 500 years. For the rock properties used in the TSw hydrogeological unit, heat pipe conditions develop above and below the repository in 10-100 years. This enhances heat transfer from the repository to the water table and to the land surface. For the 0.1 mm/year infiltration case the boiling zone is very extensive. Dry-out conditions develop and last about 2000 years in this case. At a higher infiltration rate, 4.4 mm/year , no complete dry-out zone is predicted and the liquid always flows into the repository throughout the thermal loading cycle.

This study also shows that for a 4.4 mm/year infiltration rate, the ECM and Dual-k model approaches provide similar simulation results, in terms of temperature and moisture flow and distributions. The only difference is that at the early times, the ECM model predicts more extensive boiling conditions than that from the dual-k model. This is because the ECM model simulates a "drier" repository condition.

Even though various aspect of the thermo-hydrological behavior of the mountain under thermal loading are examined in this and previous studies (Wu et al, 1995), there is still a need for more detailed investigations using a 3-D UZ model to investigate the three-dimensional effects of thermal loading. Further comparison between the ECM and the dual-k approaches may be needed in modeling studies of thermal loading effects. Based on the 2D section studies, more effort should be focused on (a) incorporating updated geological models, and fracture/matrix rock and fault properties into the 3D model; (b) coupling UZ and SZ domains; (c) a sensitivity analysis using the ECM and the dual-k models; (d) effects on ambient moisture, gas and heat flow under different infiltration scenarios; and (e) coupling site-scale with drift-scale models.

13.6 References

- Busheck T.A., and J.J. Nitao, Repository heat driven hydrothermal flow at Yucca Mountain, Part 1: modeling and analysis, Nuclear Technology Vol. 104, Dec., 1993.
- Buscheck, T.A., and J.J. Nitao, The impact of thermal loading on repository performance at Yucca Mountain, Proc. 3Rd Int. High-Level Radioactive Waste Management Conf., Las Vegas, NV, April 12-16, 1992, American Nuclear Society (1992); see also UCRL-JC-109232, Lawrence Livermore National Laboratory (1992).
ACCN: NNA.19930125.0078
- Buscheck, T.A., and J.J. Nitao, Modeling hydrothermal flow in variably saturated, fractured, welded Tuff during the prototype engineered barrier system field test of the Yucca Mountain Project, Proc. 5Th Workshop Flow and Transport Through Unsaturated Fractured Rock, Tuscon, AZ, Jan 7-10, 1991, University of Arizona; see also UCRL-ID-106521, Lawrence Livermore National Laboratory (1991).
ACCN: NNA.19911212.0238
- Flint, A.L., E.L. Flint, and J.A. Helvesi, Conceptual and numerical model of infiltration for the Yucca Mountain area, Nevada, U.S. Geological Survey, Water Resources Investigation Report-96, Denver, CO, 1996.
- Nitao, J.J., Numerical modeling of the thermal and hydrological environment around a nuclear waste package using the equivalent continuum approximation: Horizontal emplacement, UCID-21444, Lawrence Livermore National Laboratory (1988).
ACCN: NNA.19890317.0021
- Pruess K., TOUGH2 - A general purpose numerical simulator for multi-phase fluid and heat flow, Lawrence Berkeley Laboratory Report LBL-29400, Lawrence Berkeley Laboratory, Berkeley, CA; 1991.
ACCN: NNA.19940202.0088
- Pruess, K., J.S.Y. Wang, and Y.W. Tsang, On thermohydrologic conditions near high-level waste emplaced in partially saturated fractured Tuff. 1. Simulation studies with explicit consideration of fractures effects. Waste Resources Research Vol. 26 No.6, pp 1235-1248, June 1990.
ACCN: NNA.19910328.0073
- Ruffner, D., G.L. Johnson, E.A. Platt, J.A. Blink. And T. Doering, Drift emplaced waste package thermal response, Proc. 4Th High-Level Radioactive Waste Management Conf., Las Vegas, NV, April 26-30, 1993, American Nuclear Society (1993).
ACCN: NNA.19930303.0198

Ryder, E.E., Comparisons of predicted far-field temperatures for discrete and smeared heat sources, Proc 4th Int. High-Level Radioactive Waste Management Conf., Las Vegas, NV, April 26-30, 1993, American Nuclear Society (1993).

Sass J. H., A.H. Lachenbruch, W.W. Dudley, Jr., S.S. Priest, and R.J. Munroe, Temperature, thermal conductivity and heat flow near Yucca mountain, Nevada some tectonic and hydrologic implications, U.S. Geological Survey report USGS-OFR-87-649; DE89 002697, U.S. Geological Survey, 1988.

ACCN: NNA.19890123.0010

DTN: GS950408318523.001 Non-Q

TRW, Thermal loading study for FY 1995, Report B000000000-01717-5705-00016, January 31, 1996.

Witherspoon, P.A., A. Freeze, F. A. Kulacki, N. Moore, F.W. Shwartz, Y.C. Yordos, K.A. Mrotek, and R.A. Levich, Report of the thermohydrologic modeling and testing program peer review record memorandum, Yucca Mountain Project Report, 1996.

**FRACTURE COATINGS AND
FRACTURE CHARACTERISTICS WITH
IMPLICATIONS FOR FLOW
ALONG FAST PATHWAYS**

A. Simmons

August 1996

14.1 Introduction

The main parameter needed for total system performance assessment and for testing key hypotheses of the DOE Waste Isolation Strategy is percolation flux at the repository horizon. Percolation flux will be the key factor in estimating seepage into drifts, waste dissolution, and in evaluating transport along fast pathways through the unsaturated zone. A series of borehole tests in the underground Exploratory Studies Facility (ESF) is planned to attempt to derive an *in situ* estimate of percolation flux from measurement of saturation and moisture tension in cores and by direct observation. Other lines of evidence should be used to support *in situ* investigations, however, and one of these may be through the depositional record of fracture coatings. The purpose of this chapter is to summarize knowledge of fracture characteristics and fracture coatings at Yucca Mountain and to propose a means of using this information to bound uncertainties in models of percolation flux through the repository horizon.

Mineral-lined fractures provide a good record of water movement and its relation to climate variations. The U.S. Geological Survey has undertaken a program of U-series and ^{14}C dating of calcite and opal to establish a history of deposition of fracture and cavity fillings and to bound past percolation flux through the repository horizon. Los Alamos National Laboratory has examined extensive sections of borehole core to characterize the mineralogy of fracture linings, to relate mineralogy to differences in water chemistry, hydrothermal conditions, and source regions, and to assess the role of fracture coatings in retardation of radionuclides. Glassley (1995) simulated the step-wise evaporation of water under equilibrium conditions (described later in this chapter) as a preliminary estimate of how solids might precipitate along fracture walls during a thermal pulse, with consequent alteration of flow properties. The combined information from these studies has allowed us to develop an approach to modeling predicted flux through the repository horizon based on precipitation and dissolution rates of solids with interaction between rock matrix and percolating water under steady and transient conditions.

The characteristics of fractures and their coatings may provide useful parameters for calibration of the site-scale unsaturated zone flow model, whose purpose is to characterize flow pathways and processes in the unsaturated zone at Yucca Mountain [see chapter 1 of this report (Bodvarsson et al.) for a thorough description of calibration of this model]. Fracture parameters such as aperture, orientation, and density are needed in calibration of the gas flow model component (Ahlers et al., 1995, 1996). Fracture coatings are important in

investigating fracture-matrix interactions and are key considerations for permeability and for determination of flow pathways and percolation flux [see chapter 10 (Fairley et al.) and chapter 11 (Sonnenthal et al.) of this report]. As such, use of fracture characteristics as a calibration parameter may allow us in the future to discriminate among conceptual flow models and to select a preferred model. At this time, however, we intend to apply many conceptual models and will see how fracture characteristics play a role in each of them. In this chapter we summarize fracture properties, mineralization, and age dating that provide insights into percolation flux in the past. We present previous modeling results and outline a planned approach for predicting flux at the repository horizon based on current knowledge, collaboration with others studying fracture coatings, and confirmation by *in situ* tests that will be augmented by model predictions.

14.1.1 Quality Assurance Status of Data and Software Used in This Chapter

Data in this chapter are taken from several key sources and are both qualified (Q) and unqualified (non-Q). Accession numbers and data tracking numbers, when available, are provided in the reference list. Data taken from full-periphery ESF maps are preliminary (non-Q) and have not been reported to the ATDT (Beason, 1996). Fracture characteristics data of Anna (1996) are qualified. Data taken from Rousseau and others (1996) in Table 14.1 are considered qualified because they rely on qualified core from boreholes. The acquired data as reported in the ATDT were not consulted, however. Information on mineral coatings presents a gray area because much of the core originally examined (G-1, G-2, GU-3, G-4, UE-25a#1) was not qualified, but all of the x-ray diffraction and petrographic analyses conducted by Los Alamos was done under a full QA program. Other cores examined by Los Alamos (UZ-14 and UZ-16) were qualified (Carlos, 1993; 1994). Modeling results of Glassley (1995) were reported as non-Q. Groundwater composition data (Beason et al., 1993) is non-Q. Information taken from regional stress studies (Stock and Healy, 1988; Swolfs and others, 1988) is non-Q. U-series and ^{14}C ages from Paces (1996) are Q, but isotope ages taken from Szabo and Kyser (1990) are non-Q.

14.2 Fracture Distribution and Characterization

As previously stated, determination of percolation flux and knowledge of fracture-matrix interactions are important components of conceptual models of flow in the unsaturated zone at Yucca Mountain. Various aspects of the unsaturated zone flow model rely on knowledge of fracture distribution within the mountain and fracture characteristics, such as moisture tension [chapter 8 of this volume (Wu et al.)], temperature and heat flow calibration [chapter 9 (Wu et al.)], environmental isotope calibration [chapter 10 (Fairley et al.)], and thermal loading predictions [chapter 13 (Haukwa et al.)]. Characterization of fractures at Yucca Mountain has been undertaken by outcrop mapping, measurement in boreholes, and detailed mapping in the ESF. Throckmorton

and Verbeek (1995) conducted a regional study of fracture orientation on numerous outcrops, particularly the Tiva Canyon Member, at Yucca Mountain. They differentiated joints and fractures formed during initial cooling and contraction of the ignimbrite sheets from those that resulted from fracturing of the rock as a result of tectonic processes. They determined that the cooling joints either strike dominantly to the northwest (about N45°W) or to the northeast (N50°E) and dip near vertically. Along with a set of cooling joints that runs subparallel to the foliation direction of the tuff, the cooling joints form an orthogonal, three-dimensional network. Throckmorton and Verbeek (1995) also identified four sets of tectonic fractures within the North Ramp area, all of which are extensional. The first set strikes north-south and dips nearly vertically. The second set strikes northwest and generally dips steeply to the southwest. The third set strikes northeast and dips nearly vertically. The fourth set strikes east-west and is nearly vertical. Anna's (1996) characterization of fractures in the Tiva Canyon Member beyond the ESF starter tunnel showed fairly close agreement with three sets identified by Throckmorton and Verbeek (1995) as being tectonic fractures, although he did not differentiate as to whether the fracture sets were due to cooling or tectonics. One dominant orientation noted by Anna (1996) is N5°W, 76°SW; another is N54°W, 83°SW; and the third is N38°E and is vertical.

Rousseau and others (1996) indicated that the number of fracture sets and sequence of fracture formation in the Paintbrush nonwelded hydrogeologic unit (PTn) are similar to those documented for the welded units of the Paintbrush Group (Throckmorton and Verbeek, 1995). A network of cooling joints is developed where pyroclastic flows in the PTn are welded. The network consists of two orthogonal sets that are steeply dipping, and less frequently, a third subhorizontal set. A younger network of tectonic fractures consists of at least three sets of steeply dipping fractures, the oldest of which is oriented north-south, followed by northwest-trending, and then by northeast-trending sets.

Overall fracture intensity of the PTn is low and fractures are poorly connected within and between PTn lithostratigraphic units. Each of the PTn units appears to have its own fracture network with characteristic fracture spacing, intensity, and termination style; however, most of the fractures in the PTn are stratabound and terminate at welding breaks or lithologic breaks. In the ESF, PTn exposures have much lower fracture densities than observed in surface exposures (Rousseau et al., 1996). Nearly all PTn discontinuities in the ESF are minor faults with dips less than 75 degrees and slickensides that indicate predominantly dip-slip movement, most likely of tectonic origin. These planar zones are generally <4 cm wide and nearly all have thin (<0.5 cm) silica or calcite fillings (Rousseau et al., 1996). See chapter 10 of this volume (Fairley et al.) for details of effects of fracture coatings in reducing permeability through the PTn.

Fracture Coatings and Fracture Characteristics with Implications for Flow Along Fast Pathways

From detailed maps of the ESF, dominant fracture orientations were determined from equal area net plots (Beason, 1996). Within the middle non-lithophysal zone of the Topopah Spring welded unit (TSw) between stations 28+00 and 56+31, four orientations were indicated: a small set at N105°W, 20°SW; two dominant sets, one at N55°W, 83°SW, and another at N35°E, 80°NW; and a weaker set at N22°E, 80°NW. These agree quite well with the four sets of tectonic fractures identified by Throckmorton and Verbeek (1995) if the N22°E set is viewed as north-south. No dominant subhorizontal orientations were identified.

Fracture densities were averaged from histograms of boreholes USW UZ-14, USW UZ-9, USW NRG-7a, USW NRG-6, USW NRG-5, and USW NRG-4 (all in Rousseau et al., 1996). We compared this information to fracture density data determined from ESF mapping (Beason, 1996). Results are tabulated for comparison in Table 1. The borehole data show a somewhat higher fracture density in the TCw, PTn, and in the upper part of the TSw than that indicated by ESF observations, but otherwise compare quite closely. One possible way to account for this discrepancy is by different counting methods; every borehole fracture may have been counted, regardless of length, whereas some minimum cutoff length was set for fractures mapped in the ESF. Undoubtedly some fracturing of core also occurred during drilling.

Table 1.
Fracture densities (in fractures per meter) as determined from ESF and borehole data.

Stratigraphic Unit	Borehole Designators						
	ESF	UZ-14	SD-9	NRG-7A	NRG-6	NRG-5	NRG-4
Tiva: xtal-rich	1.4	-	-	-	-	-	-
Tiva: xtal poor		-	-	-	4.3	-	-
Tiva: vitric		-	9.2	0.7	6.6	-	-
Yucca Mountain	0.5	3.3	3.4	1.4	-	-	-
Bedded Tuff		1.3	-	3.3	3.4	-	0.7
Pah Canyon		0.7	0.3	1.3	1.7	-	0.7
xtal-rich vitric-TSw	3	9.2	15.8	6.6	2.6	-	3.3
u. non-lithophysal-TSw	1.8	1.3	1	5.6	9.2	-	3.3
u. lithophysal-TSw	1.4	1.7	0.7	1.7	2.6	0.7	0.7
mid non-lithophysal-TSw	4.4	4.3	3.3	4.6	5	9.9	-
lower lithophysal-TSw	-	1.4	1.7	2.3	2.6	4.6	-
lower non-lithophysal-TSw	-	4.3	6.6	4.3	-	-	-
xtal-poor vitric-TSw	-	2.8	0.4	3.3	-	-	-

Fracture Coatings and Fracture Characteristics with Implications for Flow Along Fast Pathways

Table 1.
Fracture densities (in fractures per meter) as determined from ESF and borehole data.

Stratigraphic Unit	Borehole Designators						
	ESF	UZ-14	SD-9	NRG-7A	NRG-6	NRG-5	NRG-4
Calico Hills Unit	-	0.7	1.7	-	-	-	-
Prow Pass	-	0.7	1.7	-	-	-	-
Bullfrog	-	0.7	-	-	-	-	-

1) Borehole data from Rousseau et al., 1996.
 2) ESF data from full-periphery ESF maps (Beason et al., 1996).
 3) Fractures were identified macroscopically by visual inspection.

Data from these boreholes indicate a similar trend that includes: 1) high fracture density near the contacts between vitric zones (both crystal-rich and crystal-poor) and non-lithophysal units in the TS_w; 2) relatively higher fracture density within the non-lithophysal units as compared to the lithophysal units; 3) relatively lower fracture density within the PT_n; and 4) very low fracture density within the Calico Hills Formation and the Prow Pass and Bullfrog Tuff Members of the Crater Flat Tuff.

Little information on fracture aperture distributions is available. Anna (1996) arrived at a range of apertures of 100-300 microns in the TC_w using the cubic law and 500 microns by seismic velocity calculations. (The cubic law relates the aperture of a parallel plate fracture to its effective permeability). Aperture values used in this report (chapter 11; Sonnenthal et al.) were derived from air permeability data, using 2 darcies for horizontal permeability and 10 darcies for vertical permeability. Under the infinite parallel plate model, apertures were calculated to be 200 microns, which compares well to 180 microns used in TSPA (Wilson et al., 1993). The fracture spacing then used in the percolation flux model (chapter 11) is 3-15 fractures/meter, which is close to the moving average cited by Day and Beason (1996) for ESF fractures in the TS_w. Furthermore, mineralogic data from borehole cores and the ESF substantiate the presence of wide fracture apertures in some places. In the upper lithophysal interval of the TS_w, radiating stellerite crystals indicate significant open apertures (>3 mm) in some fractures (Carlos, 1994).

We can say something about the relationship between aperture and liquid permeability based on knowledge of the stress field, on pneumatic data, and on fracture density. Studies by Stock and Healy (1988) and Swolfs and others (1988) showed that the horizontal stress field in the North Ramp study area is 25-50% less than the vertical stress field. Because of this, loading across high-angle fractures will be less than across low-angle fractures and the apertures of high-angle fractures will tend in general to be larger than the apertures of frac-

tures with low-angle orientations, resulting in higher vertical permeabilities (Rousseau et al., 1996).

In situ pressure data (Rousseau et al., 1996) showed that lithostratigraphic units could be divided into four distinct pneumatic systems: 1) the TCw; 2) the Paintbrush nonwelded (PTn) hydrogeologic unit that includes the crystal-poor vitric base of the Tiva Canyon Tuff, the Yucca Mountain and Pah Canyon Tuffs with associated bedded tuffs and the crystal-rich top of the Topopah Spring Tuff; 3) the TSw; and 4) the pre-Topopah Spring bedded tuff, nonwelded tuffs of the Calico Hills Formation, and pre-Calico Hills Formation bedded tuff (CHn). Very little phase attenuation and amplitude lagging of the pressure signal occurred in the TCw, indicating little difference between pneumatic pressure of the unit and atmospheric pressure. Pneumatic characteristics of subunits within the PTn were quite different from one location to another. Locally the pneumatic characteristics of the crystal-rich vitric zone (PTn) appear to be dominated by fracturing. Pressure data from the TSw showed negligible attenuation and lagging of the pneumatic pressure signals transmitted across the vitric PTn. Pneumatic diffusivity of the TSw unit is very high; fractures within the TSw are apparently very permeable and highly interconnected within both the lithophysal and non-lithophysal units (Rousseau et al., 1996; Ahlers et al., 1995, 1996). ESF data indicate that fracturing in the TSw repository host sequence is likely strata bound (Day and Beason, 1996). Free-draining fractures were not observed. Air permeability measurements of ≥ 10 darcies were measured in the TCw and indicate a horizontal to vertical anisotropy of 10:1 in the TCw (Day and Beason, 1996), probably due to sub-horizontal unloading fractures. In contrast, a vertical to horizontal anisotropy of 3-10:1 exists in the TSw (Day and Beason, 1996), which is partially explained by the absence of sub-horizontal orientations in this horizon.

Regression analysis by Rousseau and others (1996) indicated a small correlation between increasing fracture density and increased air permeability. Although the exact cause of the relationship is unclear, it may be a function of fracture aperture. If fracture density and permeability are correlated in this way, a few fractures with large apertures will result in a high permeability value, whereas fracture zones with many small apertures will have lower permeability. Conversely, if there is little correlation, then a few fractures with large apertures will have equivalent permeabilities to many fractures with small apertures. Individual fracture permeabilities are often controlled by aperture, which in turn is influenced by the degree of mineral coatings on fracture walls. The next section summarizes our knowledge of fracture mineralization.

14.3 Distribution and Characterization of Fracture Coatings

In this section, fracture-lining minerals are described according to their stratigraphic location at Yucca Mountain, followed by generalizations about the sequence of their formation and compositional differences above and below the water table. Special attention is then paid to calcites because of their importance in age dating and in percolation flux determination, which is the key flow parameter in the unsaturated zone flow model. The location of boreholes from which fracture coatings were characterized from core sections is shown in Figure 14.3.1.

Figure 14.3.1

Location map showing Yucca Mountain, generalized lithologic units, and drillholes mentioned in this report from which core was analyzed by Los Alamos National Laboratory (modified from Carlos et al., 1995a).

14.3.1 Stratigraphic Control

In the upper part of the TCw in UE25 UZ-16, coatings are tridymite, calcite, opal, and clay. Below this, calcite is predominant and seals some fractures. Lower still in the Tiva, opal becomes more frequent along with ubiquitous calcite, and prismatic zeolites or tridymite may coat some fractures (Carlos, 1993). In drill core from USW UZ-14, there were no coated fractures in the Pah Canyon Member (Carlos, 1994).

According to studies by Carlos and others (1995a), in the Topopah Spring Member calcite and/or opal are the most abundant fracture coatings in the first 300 feet with increasingly abundant tridymite and quartz overlain by calcite at greater depths to the base of the upper lithophysal zone. Within the lithophysal zone, prismatic heulandite or stellerite coat some fractures and in some are overlain by calcite. Below the upper lithophysal zone the dominant coatings are manganese oxides frequently overlain by zeolites (mordenite, heulandite, or stellerite). Tridymite and hematite, along with fluorite, calcite, and opal coat some lithophysal cavities. The clays smectite, palygorskite, and sepiolite are common in fractures of the Paintbrush Group in drill core USW GU-3; smectite occurs in all drill cores and ubiquitously throughout the section at Yucca Mountain but its abundance varies. It usually is a late-formed mineral. Calcite commonly appears to be the last mineral deposited wherever it occurs, and its distribution across the mountain is variable (Carlos et al., 1991). This sequence is maintained to the vitrophyre. Few coated fractures exist below the vitrophyre in the Topopah Spring Member.

14.3.2 Sequence of Coatings in TSw

The sequence of fracture coatings reveals something of water chemistry at the time of deposition and also provides insights into paleoclimate, which allows predictions to be made of future climate changes that can be used in the unsaturated zone flow model (see chapter 8 of this volume; Wu et al.). From the five drill cores USW G-1, USW G-2, USW GU-3, USW G-4, and UE-25a#1, Carlos and others (1991) derived a general sequence of mineral deposition in fractures in the devitrified tuff above the TSw vitrophyre. The first-formed fractures are connected to lithophysal cavities and originally contained tridymite, which may or may not now be transformed to cristobalite or quartz and may contain other vapor-phase minerals, e.g., hematite and/or fluorite. They appear to have been formed during degassing and devitrification of the tuff. The second fractures to form were smooth, nearly planar features which may be cooling fractures. The first coatings on these fractures are often manganese oxides that are sometimes coated with fine-grained mordenite crusts (Carlos et al., 1991). Since these fractures are often slickensided and since most of the tectonic movement at Yucca Mountain occurred prior to 10.5 Ma, it is postulated that these fractures formed prior to this time. After formation of fractures related to lithophysal cavities and planar fractures, the third type of fracture to form has rough walls without slickensides, and therefore formed after most of the tectonic activity had ended at Yucca Mountain. Coarse-grained stellerite,

heulandite, and mordenite appear to have formed after fine-grained mordenite that occurs in planar fractures.

Fracture-lining minerals in the Paintbrush Group vary both with depth and laterally across Yucca Mountain, whereas fracture coatings in tuffs below the Paintbrush Group are related to the mineralogy of the tuffs and follow a consistent pattern of distribution, with predominantly quartz, calcite, and manganese oxides in the devitrified intervals and mordenite and clinoptilolite in the zeolitic intervals minerals (Carlos et al., 1990, 1991; Carlos, 1993). Variation in zeolite fracture mineralogy can be attributed to small local differences in silica activity and chemical conditions (Chipera et al., 1993). At lower silica activities, (e.g., equilibrated with cristobalite or tridymite), stellerite and/or heulandite are most likely to form. The dominant control on heulandite vs. stellerite deposition is the concentration of dissolved cation species in the ground water (Carlos et al., 1995b), especially relative concentrations of Ca, Sr, and Mg. Furthermore, fractures in the Paintbrush Group contain a generally calcic suite of minerals, including calcite, Ca-zeolites (stellerite, heulandite, and mordenite), Ca-smectite, and Mn-oxide minerals, along with silica polymorphs. Pore water extracts from the Paintbrush Group where it is above the water table (Yang, 1992) have a different chemistry from that of groundwater from the Paintbrush Group below the water table (Benson et al., 1983), with markedly increased Ca, Mg, K, and Sr above the water table. Above the water table the Mn-oxides in fractures are principally lithiophorite, rancieite, and todorokite with exchangeable cations Na, K, Ca, Ba, and Ce (in order of abundance). Below the water table cryptomelane-group Mn-oxide minerals (cryptomelane, hollandite, coronadite) and lesser amounts of todorokite and pyrolusite occur. Exchangeable cations in this group include K, Ba, Pb, Sr, Na, and Ca. The Mn oxides are key past recorders of water-rock interaction (Vaniman et al., 1992). The contents of pore waters, compared with the composition of ground water below the water table, appear to be reflected in the fracture-lining mineral assemblages in the Paintbrush Group (Carlos et al., 1995a).

14.3.3 Calcite

Calcite occurs in many forms and in several generations throughout most strata at Yucca Mountain. For this reason, and because of the dependence on Ca concentration in groundwater with respect to formation of particular mineral species over others, calcite is the most important fracture coating to consider in calibration of the unsaturated zone flow model, with opal and silica polymorphs being second. The earliest-formed calcite is the most abundant calcite in the tuffs; it occurs in fractures, in faults, in the matrix, and as pseudomorphs of feldspar phenocrysts in deep intervals where hydrothermal alteration of 10.7 Ma is preserved (Bish, 1989). Calcite is generally found at shallower depths at Yucca Mountain only within fractures and as a late precipitate within lithophysal cavities. Calcites deposited in fractures above the water table have a broad range of ages; U-series ages of 26 to >400Ka have been obtained, and ^{14}C ages cluster between 33-45 Ky (Szabo and Kyser, 1990). Both

the U-series ages and the observed fracture-coating mineral sequences (Carlos et al., 1991) indicate that calcite is usually the latest formed authigenic mineral above the water table.

Szabo and Kyser, (1990) also analyzed opals and found that all gave U-series ages of >400Ka; however, fracture mineralogy studies (Carlos et al., 1991) show that some opal deposits formed on top of some calcites. The parageneses of fracture deposition suggest that calcite and opal may have been deposited under a variety of conditions beginning soon after tuff emplacement, but that deposition of calcite and perhaps opal continued during Pleistocene episodes of greater flow through the unsaturated zone and may be, at least with respect to calcite, continuing under present conditions (Vaniman et al., 1992).

Vaniman and Whelan (1994) noted a strong genetic connection between calcretes formed at the surface and calcites deposited in underlying fractures in the unsaturated zone. Szabo and Kyser (1990) suggested from stable isotope data that the coarser-grained calcites deposited in unsaturated fractures over the last 400 Ka formed from meteoric waters. Unsaturated zone calcite $\delta^{13}\text{C}$ values indicate input of pedogenic carbon, and $^{87}\text{Sr}/^{86}\text{Sr}$ increases from shallow ground water ratios near the water table to pedogenic values near the surface (Marshall et al., 1992). Whether all calcites and opal in unsaturated fractures were precipitated from solutions transported from the surface is unknown, but it is possible that downward transport was involved in the formation of the chain-structure clays, sepiolite, found in fractures as deep as 146 m, and palygorskite, found in fractures as deep as 253 m (Carlos et al., 1991; Vaniman et al., 1992).

14.4 Flux

As stated previously, stable isotope data indicate that the low-temperature calcite and opal deposits filling fractures and cavities at Yucca Mountain were deposited by meteoric waters percolating through the unsaturated zone. The coatings contain information about the times of deposition (U-series and ^{14}C) and the isotopic character of the waters from which they precipitated ($\delta^{13}\text{C}$, $\delta^{18}\text{O}$, $\delta^{87}\text{Sr}$, $^{234}\text{U}/^{238}\text{U}$). The mass of calcite and opal per unit volume of host rock may be related to the past water flux which transported the ions to sites where they precipitated from solution, possibly under evaporative conditions. Because it is known that the water table elevation varied by as much as sixty meters under wetter paleoclimatic conditions at Yucca Mountain (Levy, 1991), precipitation of minerals under unsaturated conditions must be demonstrated in order for assumptions of evaporative deposition to be valid. This demonstration has yet to be made rigorously, but mineral textures suggest that crystals grew in open spaces rather than under saturated conditions.

Paces (1996) sampled two types of secondary coatings in the ESF: 1) coatings lining steep-to shallow-dipping fractures and fracture zones (typically present on the footwall), and 2) mineral-coated floors of open lithophysal cavities that are typically intersected by narrow aperture fractures. Traces of major faults in the ESF (Bow Ridge, Drillhole Wash, and Sundance) are not mineralized. The lithophysal cavities typically contain a thin rim of high-temperature, vapor-phase minerals (tridymite +/- hematite) formed during cooling immediately following emplacement of the tuffs that are often overlain by coatings of calcite and silica representing deposition from low-temperature aqueous solutions. The form of silica near the base of the coatings is commonly non-layered to massive, where present, and is composed of undifferentiated quartz and chalcedony, with minor opal on or near the outermost, free-face calcite surfaces. Opal forms the latest depositional event on some samples and on others shows evidence of calcite overgrowths (Paces, 1996). Calcite constitutes the bulk of the volume of most occurrences, generally as even coatings of equigranular blocky prisms to thin, upright and sometimes large (≥ 2 cm) "blades" (Paces, 1991).

Steeply dipping fracture occurrences generally contain calcite, locally overlying earlier massive silica deposits. In fractures containing open space, which occur commonly and sometimes have centimeter-scale apertures (Paces, 1996), mineral deposition is preferentially located on the footwall with a complete absence of calcite on the hanging wall. Tall calcite blades and bubbly or laminated opal common to lithophysal cavities are unusual in steeply dipping fractures. Layering of the calcite and opal coatings indicate that mineral growth occurred progressively outward from the tuff matrix substrate into open space, which provides evidence of unsaturated conditions during mineral growth. Paces (1996) found no obvious differences in age between lithophysal cavity and fracture-filling occurrences. Therefore, the lithophysal cavities would be just as likely to experience percolation of water as the fracture pathways. Furthermore, the data suggest a crude correlation between decreasing isotopic age of fracture coatings and increasing depth in the ESF (Paces, 1996), which suggests the deposition of material from younger waters at greater depth, and may provide corroborating evidence for rapid percolation flux along fast pathways.

Preliminary data indicate that calcite and opal are not common in discrete zones which contain bomb-pulse ^{36}Cl (Peterman and Paces, 1996), but are consistent with slow percolation through the rock mass. They determined U-series ages of opal and calcite ranging from 37 to >500 Ky. ^{14}C ages of calcite range from 16 to >40 Ky. Peterman and Paces (1996) reasoned that calcite and opal were deposited under unsaturated conditions in which fractures and cavities were not filled with water, because deposition requires open space for evaporative concentration, but evaporative concentration has not been demonstrated conclusively. Typically the calcite and opal occur in fractures and cavities with openings greater than several millimeters. In single fractures with variable openings, narrow intervals contain little or no mineralization whereas wider zones are mineralized. Deposits are thicker and more complex on low-angle

features. Mineral textures suggest low-volume water films migrating down fracture surfaces into cavities. Isotopic exchange with the tuff matrix, as shown in $\delta^{13}\text{C}$ and $\delta^{18}\text{O}$ ratios, indicates modification of infiltrating water during percolation by rock-water interaction. Rock-water interaction may be unlikely under evaporative conditions, but rock-matrix interaction is a plausible mechanism for concentrating solutions to supersaturation and precipitation. According to Peterman and Paces' (1996) mass balance calculations, depositional rates were slow, on the order of micrometers per thousands of years, indicating low flux.

Crystal growth may be continuous over long time periods or may terminate, only to begin at a later time when conditions change. The growth rate is an important factor to consider in estimating percolation flux, but sampling methods often require material with different ages and isotopic apparent ages may not accurately reflect a single date. Whether or not an isotopic analysis represents an individual layer depends on the layer thickness and ability of the sampler to discriminate between layers. To address the issue raised by sampling, and the fact that measured isotopic ratios are dependent on sample thickness and growth rate, Peterman and Paces (1996) arrived at two end-member conceptual models to explain percolation flux based on mineral coating data, one in which continuous deposition occurs and one in which deposition is episodic (see Figure 14.4.1). Their continuous deposition model (Figure 14.4.16) assumes that growth of secondary minerals has occurred at a constant, but extremely low rate resulting in a continuum of infinitely thin layers. In the continuous deposition model, the isotopic ratio represents multiple layers so that the calculated age reflects a mixed age intermediate between the age of the outermost and innermost layers. When secondary mineral growth is very slow, younger ages will be obtained for smaller samples from the same surface and isotopes with shorter half-lives will yield younger calculated ages for the same material.

Figure 14.4.1

Schematic of two conceptual models of percolation flux developed by U.S. Geological Survey and based on mineral coating apparent ages (from Peterman and Paces, 1996). t = relative time of deposition of layers. a) episodic/instantaneous model; b) continuous deposition model.

If mineral deposition is episodic or instantaneous (Figure 14.4.1a), discrete mineral layers form over time intervals that are brief relative to the half-lives of the isotopic dating methods being used, and deposition is rapid relative to the interval between events. In this situation, measured isotopic ratios are uniform because the isotopic analysis represents a single layer, so that the calculated age represents the age of the discrete depositional event, and different isotopic clocks will record concordant ages for the same materials analyzed.

Natural systems of mineral deposition may experience periods of both rapid, episodic mineral growth as well as more continuous growth periods. However, data collected from ESF secondary mineral deposits are grossly consistent with the concept of continuous deposition, including both U-series and ^{14}C ages of outermost materials. Therefore, calculated ages are likely to reflect a mixture of ages of older and younger materials. As sampling methodology is refined and analyzed layers become smaller, apparent ages will more closely approximate actual intervals of deposition.

An understanding of depositional modes is critical for defining the style of percolation and secondary mineral deposition, as well as for addressing the connection between fracture-filling histories and time-dependent climate-based infiltration. These are important parameters for determining percolation flux. The implied flux would be substantially lowered under conditions of continuous deposition because the depositional record is extended over a much greater time interval.

14.5 Simulations of Formation of Fracture Coatings

Mineral coatings may form on fracture walls by different mechanisms depending on whether conditions are saturated or unsaturated. The relative importance of different mechanisms causing precipitation needs to be evaluated. Evaporation of water is one important consideration for establishing the nature of secondary precipitates. The solids that may develop will reflect the initial composition of water evaporated. Interaction of water with the rock matrix will tend to alter the initial composition with increasing time along the flow path. Little modeling has been done in this area in the Yucca Mountain Project to date, but as an initial attempt to investigate the effects of evaporation on the composition of precipitates that could form, Glassley (1995) considered scenarios in which water evaporation began with J-13 well water, a water that is close to equilibrium with New Zealand high-silica rhyolite similar in composition to that at Yucca Mountain (Bruton et al., 1993). J-13 was chosen as an initial bounding composition without consideration of rock-water interaction; more realistically, water flowing along fractures will experience some degree of interaction with surrounding rock that will modify its composition. However, these preliminary simulations applied to an extreme case in which evaporation occurs at high rates relative to dissolution or precipitation of rock components.

The evaporation of water was simulated using the EQ3/6 code (Wolery, 1992 a, b; Wolery and Daveler, 1992) by removing water at a specified rate during reaction progress in an EQ6 simulation. J-13 water was evaporated at constant temperatures of 31°C and 90°C as well as at increasing temperatures between 31°C and 90°C using arbitrary relationships between amount of water evaporated and temperature change. Phases that precipitated included calcite, dolomite, silica polymorphs, saponite, and stilbite, as well as minor quantities of low-solubility fluorapatite, nontronite, and pyrolusite. Glassley's (1995) simulation results showed that the most significant variable controlling evolution of the water chemistry and the solids that precipitate is the composition of the coexisting gas phase (CO_2 and O_2) and whether gas and water are in equilibrium. This can be seen in the divergence of pH and Eh as evaporation proceeds in both cases. When the gas composition is fixed, pH and Eh vary inversely, whereas when CO_2 and O_2 are not fixed and the system is open, pH decreases and Eh increases due to changes in oxygen partial pressure. These effects influence total concentration of elements that occur in silicates and carbonates that have solubilities sensitive to moderate changes in solution pH. Further modeling under evaporative conditions should consider the consequences of reacting Topopah Spring Tuff with evaporating waters and should consider waters of various compositions, such as unsaturated zone pore water, perched water and saturated zone water. Additional modeling should consider precipitation mechanisms other than evaporation.

14.6 Uncertainties

The estimation of percolation flux from apparent ages of fracture coating minerals and from deposition models is a useful approach, but as with any approach, it carries associated uncertainties that must be remembered and accounted for. First, the possibility of dissolution of mineral coatings under wetter conditions must be accounted for, both in reaction-path models and in apparent age models. Paces (1996) looked for (but found little) evidence of dissolution in mineral textures and in U-series disequilibrium systematics with formation of thorium. In addition, as calculated ages approach the upper limits of an isotopic clock, the less capable they are of resolving age information for the material sampled.

One of the most important uncertainties to account for is the channelized nature of flow. The channelized nature of flow makes predictions of percolation flux integrated over the site a more difficult challenge than flux along a single fracture. *In situ* tests designed to address this problem are planned for the period of performance confirmation testing after the 1998 Viability Assessment. These tests will draw on numerous additional lines of evidence to determine flow. They will also test the travel time and pathway of water flowing through fractures. Thoma and others (1992) have shown that the existence of fracture coatings could significantly decrease the travel time and increase the travel depth of water flowing through fractures. If a fracture face is not coated, water can be imbibed across it into the adjacent porous matrix by capillary suction forces, once fracture flow has begun. However, if flow across the fracture face is inhibited by coatings or some other means, then flow down the fracture face could continue. The amount of water retained by the fracture will depend on the properties of the fracture, the matrix, and the fracture/matrix interface, in addition to the matrix saturation and the magnitude and duration of the infiltration event. Tokunaga and Wan (in press) measured the hydraulic conductivity of an unconfined block of Bishop Tuff over a range of near-zero matric pressure potentials. They demonstrated the capacity of natural, rough surfaces to conduct water at high velocities and under tension and showed that surface film flow, in addition to aperture contributions, may help explain observations of short travel times for solutes transported to deep, unsaturated fractured rock. Simulation of formation of fracture coatings as discussed in the next section should also help to estimate percolation flux by bounding scenarios for formation of coatings and may help to reduce uncertainties in the unsaturated zone flow model).

14.7 Summary and Recommendations

Fracture characteristics such as orientation, density, size, connectivity, aperture, and mineral linings are important parameters for calibration of the unsat-

urated zone site-scale flow model because they relate to fracture permeability and may be able to tell something about percolation flux. In addition, fracture characteristics are important to understanding fracture-matrix interactions, which play a role in selection of conceptual flow models (e.g., equivalent continuum, dual-porosity-dual permeability), and provide important constraints on travel-times along pathways (i.e. film flow along coated fractures may be much more rapid than along uncoated fractures).

ESF mapping has begun to improve our information base on fracture characteristics, particularly in three dimensions, but more data on fracture apertures, length, tortuosity, and connectivity are needed. The project has a good information base on fracture coatings and sequence of formation (from both Q and non-Q core), with some insights as to differences in paleoclimate conditions, hydrothermal alteration, groundwater chemistry, and silica activity that were likely responsible for producing variations in mineral coating composition. Calcite is the latest mineral to form, although it may also have formed during early episodes of deposition and is the mineral most likely to form fracture coatings under present conditions (This statement is based on non-Q data but is believed to be scientifically valid). Opal is also widely distributed along fractures and lithophysae and the potential for its deposition under present conditions needs to be investigated and modeled more thoroughly. U-series and ^{14}C apparent age dating by the U.S. Geological Survey (Peterman and Paces and associates) has led to the construction of two conceptual models of episodic and continuous deposition of calcite and opal (non-Q) that provide simple bounding conditions for evaporative precipitation which may help to constrain percolation flux through Yucca Mountain. Their models appear to be more consistent with a low flux concept over long time periods, whereas other models [i.e. film flow, insights from environmental isotopes and perched water occurrence and composition discussed in chapter 10 of this volume (Fairley et al.) and percolation flux modeled in chapter 11 of this volume (Sonnenthal et al.)] are more consistent with rapid flux along preferential fast pathways. It is likely that more than one flow regime, and perhaps at least three, exists at Yucca Mountain, and the relative contribution of each should be evaluated in terms of performance assessment (this statement is non-Q).

Bearing in mind the uncertainties (discussed previously) that are inherent in estimating flux from fracture coating apparent ages, the Yucca Mountain Project should continue to explore various models of precipitation, including those due to evaporation and supersaturated conditions, as well as examine models that account for dissolution and re-precipitation of mineral coatings. Reaction-path modeling using realistic water and mineral compositions along with rock-water interaction, and accounting for relative humidity/evaporative conditions in fractures, should help to constrain the physical and chemical conditions necessary for deposition of materials along fracture walls. This information can then be used in predictions of future conditions (e.g. plugging or opening of fractures under a thermal regime with attendant changes in perme-

ability) and predictions of percolation flux that can be used in calibration of the unsaturated zone flow model in conjunction with travel-time of environmental isotopes, moisture balance, and future climate.

14.8 References

- Ahlers, C.F., T.M. Bandurraga, G.S. Bodvarsson, G. Chen, S. Finsterle, and Y.S. Wu, Summary of model calibration and sensitivity studies using the LBNL/USGS three-dimensional unsaturated zone site-scale model, Yucca Mountain Project Milestone 3GLM107M, Lawrence Berkeley Laboratory, Berkeley, CA, 1995.
ACCN: MOL.19960208.0091-0097
DTN: LB092995312293.001 Non-Q
- Ahlers, C.F., C. Shan, C. Haukwa, A.J. B. Cohen, and G.S. Bodvarsson, Calibration and prediction of pneumatic response at Yucca Mountain, Nevada using the LBNL/USGS three-dimensional site-scale model of the unsaturated zone, Yucca Mountain Project Milestone OB12M, Lawrence Berkeley Laboratory, Berkeley, CA, 1996.
- Anna, L., Preliminary three-dimensional discrete fracture model, Tiva Canyon tuff, Yucca Mountain area, Nye County, Nevada, U. S. Geological Survey Water-Resources Investigation Report, Denver, CO, (draft).
DTN: GS960408312281.001 Q
- Beason, S., ESF, North Ramp and Main Drift, full-periphery geotechnical maps for stations 00+60 to 30+00, U.S. Bureau of Reclamation/U.S. Geological Survey (preliminary), Denver, CO, 1996.
- Benson, L.V., J.H. Robison, R.K. Blankennagel, and A.E. Ogard, Chemical composition of ground water and the locations of permeable zones in the Yucca Mountain area, Nevada, U.S. Geological Survey Open-File Report 83-854, Denver, CO 1983.
DTN: GS930308312323.001 Non-Q
- Bish, D.L., Evaluation of past and future alterations in tuff at Yucca Mountain, Nevada, based on the clay mineralogy of drill cores USW G-1, G-2, and G-3, Los Alamos National Laboratory Report, LA-10667-MS, Los Alamos National Laboratory, Los Alamos, NM, 1989.
ACCN: NNA19890126.0207
- Carlos, B.A., Preliminary description of fracture-lining minerals in drill core UE25 UZ-16, Yucca Mountain Project Milestone 4013, Los Alamos National Laboratory, Los Alamos, NM, 1993.
- Carlos, B.A., Preliminary description of fracture-lining minerals in drill core USW UZ-14, Yucca Mountain Project Milestone 4005, Los Alamos National Laboratory, Los Alamos, NM, 1994.

Fracture Coatings and Fracture Characteristics with Implications for Flow Along Fast Pathways

Carlos, B.A., D.L. Bish, and S.J. Chipera, Manganese oxide minerals in fractures of the Crater Flat Tuff in drill core USW-G-4, Los Alamos National Laboratory Report LA-11787-MS, Los Alamos National Laboratory, Los Alamos, NM, 1990.

ACCN: NNA.19900206.0163

DTN: LA00000000039.001 Non-Q

Carlos, B.A., D.L. Bish, S.J. Chipera, and S. Craven, Fracture-lining manganese oxide minerals in a silicic tuff, *Chemical Geology* 107, pp. 47-69, 1993.

ACCN: NNA.19931028.0002

Carlos, B.A., D.L. Bish, and S.J. Chipera, Fracture-lining minerals in the lower Topopah Spring Tuff at Yucca Mountain, *Proceedings of the Second International High Level Radioactive Waste Management Conference*, Las Vegas, Nevada, April 28-May 3, 1991, American Nuclear Society, La Grange Park, IL, pp. 486-493, 1991.

ACCN: NNA.19910206.0039

Carlos, B.A., S.J. Chipera, and D.L. Bish, Distribution and chemistry of fracture-lining minerals at Yucca Mountain, Nevada, Los Alamos National Laboratory Report LA-12977-MS, UC-814, Los Alamos National Laboratory, Los Alamos, NM, 1995a.

Carlos, B.A., S.J. Chipera, and Snow, Multiple episodes of zeolite deposition in fractured silicic tuff, Los Alamos National Laboratory Report MS4079, Los Alamos National Laboratory, Los Alamos, NM, 1995b.

Chipera, S.J., D.L. Bish, and B.A. Carlos, Equilibrium modeling of the formation of zeolites in fractures at Yucca Mountain, Nevada, paper presented at Zeolite 1993 Conference, Boise, ID, June 20-28, 1993.

ACCN: HQO.19940518.0009

Day, W. and S. Beason, Geological structure at Yucca Mountain, presentation given to U.S. Nuclear Waste Technical Review Board, Denver, CO, July 9-10, 1996.

Glassley, W.E., Report on near-field geochemistry: water composition changes due to evaporation, Yucca Mountain Milestone MOL26, Lawrence Livermore National Laboratory, Livermore, CA, 1995.

Marshall, B.D., J.F. Whelan, Z.E. Peterman, K. Futa, S.A. Mahon, and J.S. Stuckless, Isotopic studies of fracture coatings at Yucca Mountain, Nevada, USA, in *Rock-Water Interaction, Proceedings of the Seventh International Symposium on Water-Rock Interaction*, WRI-7, Park City, Utah, July 13-18, 1992, A.A. Balkema, Rotterdam and Brookfield, Capetown, South Africa, pp. 737-740, 1992.

ACCN: NNA.19921029.0034

Fracture Coatings and Fracture Characteristics with Implications for Flow Along Fast Pathways

- Paces, J. B., Memorandum to R.W. Craig dated February 23, 1996 concerning "Submission of Milestone 3GQH455", 1996.
DTN GS960208315215.001 Q
- Peterman, Z.E. and J.B. Paces, Paleohydrology - age control from U-series and ¹⁴C dating of calcite and opal in the ESF, presentation given to U.S. Nuclear Waste Technical Review Board, Denver, CO, July 9-10, 1996.
- Rousseau, J. P., E.M. Kwicklis, and D.C. Gillies, Hydrogeology of the unsaturated zone, North Ramp area of the Exploratory Studies Facility, Yucca Mountain, Nevada, U. S. Geological Survey Water Resources Investigations Report, Denver, CO, 1996 (draft).
- Stock, J.M., and J.H. Healy, Stress field at Yucca Mountain, Nevada, in Carr, M.D., and Yount, J.C., eds., Geologic and hydrologic investigations of a potential nuclear waste disposal site at Yucca Mountain, southern Nevada, U. S. Geological Survey Bulletin 1790, Denver, CO, pp. 87-93, 1988.
ACCN: NNA.19940318.0075
DTN: GS930283117481.001 Non-Q
- Swolfs, H.S., W.Z. Savage, and W.L. Ellis, An evaluation of the topographic modification of stresses at Yucca Mountain, Nevada, in Carr, M.D., and Yount, J.C., eds., Geologic and hydrologic investigations of a potential nuclear waste disposal site at Yucca Mountain, southern Nevada, U. S. Geological Survey Bulletin 1790, Denver, CO, pp. 95-101, 1988.
ACCN: NNA.19920407.0019
DTN: GS930483117481.002 Non-Q
- Szabo, B.J., and T.K. Kyser, Ages and stable-isotope compositions of secondary calcite and opal in drill cores from Tertiary volcanic rocks of the Yucca Mountain area, Nevada, Geological Society of America Bulletin 102, pp. 1714-1719, 1990.
ACCN: NNA.19910225.0068
DTN: GS930108315215.010 Non-Q
- Throckmorton, C.K., and E.R. Verbeek, Joint networks in the Tiva Canyon and Topopah Spring tuffs of the Paintbrush Group, southwestern Nevada, U.S. Geological Survey Open-File Report 95-2, Denver, CO, 1995.
- Tokunaga, T.K., and J. Wan, Water film flow along surfaces of porous rock, Lawrence Berkeley Laboratory Report, Berkeley, CA, 1997 (draft).
- Thoma, S.G., D.P. Gallegos, and D.M. Smith, Impact of fracture coatings on fracture/matrix flow interactions in unsaturated porous media, Water Resources Research 28, pp. 1357-1367, 1992.

Fracture Coatings and Fracture Characteristics with Implications for Flow Along Fast Pathways

- Vaniman, D.T., and J.F. Whelan, Inferences of paleoenvironment from petrographic, chemical, and stable-isotope studies of calcretes and fracture calcites, Proceedings of the Fifth International High Level Radioactive Waste Management Conference, Las Vegas, Nevada, May 22-26, 1994, American Nuclear Society, La Grange Park, IL, pp. 2730-2737, 1994.
ACCN: NNA.19940607.0171
DTN: LA000000000000075.001 Q
- Vaniman, D.T., D.L. Bish, M.H. Ebinger, and S.J. Chipera, Precipitation of calcite, dolomite, sepiolite, and silica from evaporated carbonate and tuffaceous waters of southern Nevada, in Water-Rock Interaction, Proceedings of the Seventh International Symposium on Water-Rock Interaction, WRI-7, Park City, Utah, July 13-18, 1992, A.A. Balkema, Rotterdam and Brookfield, Capetown, South Africa, pp. 687-692, 1992.
ACCN: NNA.19930105.0015
- Wilson, M.L., J.H. Gauthier, R.W. Barnard, G.E. Barr, H.A. Dockery, E. Dunn, R.R. Eaton, D.C. Guerin, N. Lu, M.J. Martinez, R. Nilson, C.A. Rautman, T.H. Robey, B. Ross, E.E. Ryder, A. R. Schenker, S.A. Shannon, L.H. Skinner, W.G. Halsey, J. Gansemer, L.C. Lewis, A.D. Lamont, I.R. Triay, A. Meijer, and D.E. Morris, Total system performance assessment for Yucca Mountain - SNL Second Iteration (TSPA-1993), Sandia National Laboratories Report SAND93-2675, Sandia National Laboratories, Albuquerque, NM, 1994.
ACCN: NNA.19940112.0123
- Wolery, T.J., EQ3/6, A software package for geochemical modeling of aqueous systems: package overview and installation guide, UCRL-MA-110662, Pt. 1, Lawrence Livermore National Laboratory Report, Livermore, CA, 1992a.
ACCN: NNA.19921023.0028
- Wolery, T.J., EQ3NR, A computer program for geochemical aqueous speciation-solubility calculations: theoretical manual, user's guide, and related documentation, UCRL-MA-110662, Pt. III, Lawrence Livermore National Laboratory Report, Livermore, CA, 1992b.
ACCN: NNA.19921218.0010
- Wolery, T.J., and S.A. Daveler, EQ6, a computer program for reaction path modeling of aqueous geochemical systems: theoretical manual, user's guide, and related documentation (version 7.0) UCRL-MA-110662, Pt. 1V, Lawrence Livermore National Laboratory Report, Livermore, CA, 1992.
ACCN: NNA.19930127.0030
- Yang, I.C., Flow and transport through unsaturated rock -- data from two test holes, Yucca Mountain, Nevada, Proceedings of the Third International High Level Radioactive Waste Management Conference, Las Vegas, Nevada, April 12-16, 1992, American Nuclear Society, La Grange Park, Illinois, pp. 732-737, 1992.
ACCN: NNA.19930112.0137
DTN: GS920908312272.011 Non-Q

Participant M&O
Database - PACSYMP96
Prepared - 19-DEC-95:13:46:03

Yucca Mountain Site Characterization Project
Planning and Control System (PACS)
Participant Planning Sheet (PSA03)

Page - 1
Inc. Dollars in Thousands (Esc.)

P&S Account - 1.2.3.3.1.2.9 M&O
P&S Account Title - Site Unsaturated Zone Modeling and Synthesis
PWBS Element Number - 1.2.3.3.1.2.9
PWBS Element Title - Site Unsaturated Zone Modeling and Synthesis

Baseline Start - 01-oct-1995
Baseline Finish - 30-sep-1996

RLP 1/12/96

	Prior	FY1996	FY1997	FY1998	FY1999	FY2000	FY2001	FY2002	FY2003	FY2004	FY2005	At Future Complete
Annual Budget	0	854 589	0	0	0	0	0	0	0	0	0	0 854 589

Statement of Work *ARV 1/12/96*

1/12/96

The following quality affecting work shall be controlled in accordance with approved implementing procedures identified on the current OCRWM-accepted Requirements Traceability Network Matrix *ARV*

Select and verify computer codes that will be used to simulate specific elements of the conceptual model of the unsaturated-zone hydrogeologic system. Select appropriate code-verification and model-validation and testing exercises to be performed. Document Code. Construct two-and-three dimensional, two-phase, couples heat and moisture flow models for variably saturated, variably fractured porous media. Define hydrogeologic boundary and initial conditions. Collect, evaluate and compile hydrologic, thermal, mechanical properties for the site unsaturated zone. Conduct baseline analyses. *Perform predictive calculations of the induced effect of the excavation of the Exploratory Studies Facility on ambient conditions of the unsaturated zone. ARV*
WARD applies to this effort.

Participant agrees to perform tasks and activities as described in subordinate FY96 Summary Accounts.

1/12/96

DELIVERABLES

Deliv ID	Description/Completion Criteria	Due Date
OB02	Synthesis of Unsat-Zone Flow & Modeling YM Area Criteria - This deliverable will be the Intermediate Unsaturated-Zone Site-Scale Model and will contain the model code, a discussion of the inputs and outputs, a discussion of the calibration using data from the natural environment, and a discussion of its possible uses and limitations. The deliverable will discuss the conceptual model upon which the Site-Scale Model is based, and presents the results of hydrological data parameter analyses for data used in the model preparation. It will present the assumptions used in the model preparation, and describe the results of the calibration efforts for the important model components such as moisture flow, and heat flow. The verification and sensitivity analyses performed with the model will be summarized, especially with regard to assumed boundary conditions, fault properties, fracture properties, and hydrological parameter variation. Predictions of the borehole and Exploratory Studies Facility state variables made by the model will be compared with measured data from project scientists. The data, analysis, and conclusions from Level 3 milestone 3GUF604M and Level 4 milestone 3GUM611M due 31 May 1996, which will describe the methodology, assumptions, data on which the intermediate site scale UZ model is based, inferred model parameters, calculated fluid fluxes and moisture distribution, and calibration and verification of the site unsaturated zone hydrology	30-aug-1996
OB12M	(see description of this additional Level 3 deliverable on attached page) <i>ARV</i> <i>1/12/96</i>	30-aug-1996

Participant M&O
Database - PACSYMP96
Prepared - 19-DEC-95:13:46:03

Yucca Mountain Site Characterization Project
Planning and Control System (PACS)
Participant Planning Sheet (PSA03)

Page - 2
Inc. Dollars in Thousands (Esc.)

TR33129 Site Unsaturated Zone Modeling and Synthesis (continued)

Approvals

Larry R. Hayes
Preparer - print name

01/12/96
Date

Dennis R. Williams
Technical Reviewer - print name

1/16/96
Date

Richard A. Kettell
QA Reviewer - print name

1/13/96
Date

Larry R. Hayes
Preparer - signature

Dennis R. Williams
Technical Reviewer - signature

Richard A. Kettell
QA Reviewer - signature

WBS 1.2.3.3.1.2.9 Site Unsaturated Zone Modeling and Synthesis

Summary Account: TR33129EBK Predictive Calculations of Pneumatic Response Near the Exploratory Studies Facility (CRWMS M&O)

- **Title:** Forward Calculations of Pneumatic Response near the Exploratory Studies Facility

Deliverable No.: 0B12M

Due Date: August 30, 1996

Milestone Level: 3

Acceptance Criteria: A letter report will be prepared describing the results of the model simulations, comparisons with measured data in monitoring boreholes, and improved estimations of bulk pneumatic and hydrologic properties, including an assessment of model and data uncertainties. An evaluation based on the modeling results of the water balance in the rock mass near the Exploratory Studies Facility will be provided. The stratigraphy used in the report will be consistent with the Reference Information Base Section 1.12(a), "Stratigraphy: Geologic/Lithologic Stratigraphy" and the Prototype Three-Dimensional Framework Model (YW85) of September 1995. The use of Q and non-Q data in the deliverable will be clearly identified. Record accession numbers and Automated Technical Data Tracking numbers will be included, as appropriate, for all data used and/or cited in the deliverable. The deliverable will be submitted to YMSCO in accordance with YAP 5.1Q.