INTRAVAL Phase II Model Testing at the Las Cruces Trench Site

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MASTER

Abstract

Several field experiments have been performed by scientists from the University of Arizona and New Mexico State University at the Las Cruces Trench Site to provide data to test deterministic and stochastic models for water flow and solute transport. These experiments were performed in collaboration with INTRAVAL, which is an international effort toward the validation of geosphere models for the transport of radionuclides. During Phase I of INTRAVAL, qualitative comparisons between experimental data from two experiments (denoted Plot 1 and 2a experiments) and model predictions were made using contour plots of water contents and solute concentrations. Detailed quantitative comparisons between the predictions and field observations and between the predictions of all of the models were not made.

To provide data for more rigorous model testing, a third Las Cruces Trench experiment (denoted the Plot 2b experiment) was designed by scientists from the University of Arizona and New Mexico State University. Modelers from the Center for Nuclear Waste Regulatory Analysis, Massachusetts Institute of Technology, New Mexico State University, Pacific Northwest Laboratory, and the University of Texas provided predictions for water flow and tritium transport to New Mexico State University for analysis. The corresponding models assumed soil characterizations that ranged from uniform and isotropic, to two-dimensional heterogeneous, to stochastic. This report presents detailed qualitative and quantitative comparisons between the model predictions and field observations for the Plot 2b experiment.

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Foreword

This technical report was prepared by New Mexico State University, a subcontractor to the University of Arizona under their research project with the Waste Management Branch in the Office of Nuclear Regulatory Research (FIN L1286). The report outlines comparison strategies and results for field testing and evaluation of unsaturated flow and transport models using water flow and tracer experimental data from the Las Cruces Trench Facility. This document also serves as an INTRAVAL* Report for

presenting model testing methodology and model comparison results.

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* INTRAVAL is an international cooperative project for studying validation of geosphere transport models. Professor Richard Hills, New Mexico State University, served as the INTRAVAL Pilot Team leader in reporting on the Las Cruces Trench experiments, model testing methodology, and comparisons of models provided by other INTRAVAL modeling teams.

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1 Introduction

To provide regulatory guidance and to assist in the development of low-level waste disposal facilities, the United States Congress passed the Low Level Waste Act of 1986. As a result, a requirement for the licensing of near surface low-level waste (LLW) disposal sites, as set forth in the U.S. Nuclear Regulatory Commission (USNRC) regulations (Subpart D of 10 CFR Part 61), is that it "shall be capable of being characterized, modeled, analyzed, and monitored". One of the major environmental considerations in choosing and engineering a LLW site is the ability to predict and control the transport of LLW materials to the environment through local geological features. LLW materials that leak from their containment can reach the groundwater due to deep percolation (recharge), can be taken up by plant roots, and can be released into the atmosphere through evaporation and transpiration.

The successful estimation of the concentrations of LLW materials that reach the atmosphere, plant and animal life, and the groundwater at a particular site are hampered by the complex nature of transport through the vadose zone. While many of the physical processes that control transport are well understood on the laboratory scale, our ability to model these processes on the field scale has not been established. Data to test water flow and transport models and to test site characterization and measurement methodologies must come from well-characterized, well-monitored, and well-controlled field experiments.

With these requirements in mind, scientists from Pacific Northwest Laboratory (PNL), Massachusetts Institute of Technology (MIT), the University of Arizona (UA), and New Mexico State University (NMSU) have designed and

constructed, with support from the U.S. Nuclear Regulatory Commission (USNRC), a test facility at the New Mexico State University College Ranch northeast of Las Cruces, New Mexico. The Las Cruces Trench Site is designed to study field scale flow and transport in undisturbed, highly variable, unsaturated soils. Two test plots have been heavily instrumented with multi-dimensional arrays of neutron probe access tubes, tensiometers, and solution samplers to monitor water flow and solute transport. Water containing tracers was applied to the surface in a carefully controlled fashion during 3 experiments and the response of the system to this input observed. Soil samples from approximately 600 locations were taken from an area immediately adjacent to the test plots to characterize the important hydraulic parameters of the site.

Here we compare field observations of water flow and tritium transport to model predictions for the third experiment (the Plot 2b experiment). Water content predictions for this experiment were provided by the Center for Nuclear Waste Regulatory Analysis (CNWRA), Massachusetts Institute of Technology, New Mexico State University, Pacific Northwest Laboratory, and the Bureau of Economic Geology (BEG) at the University of Texas. Solute transport predictions were provided by New Mexico State University and Pacific Northwest Laboratory. A detailed description of the experimental procedures used for this experiment and the resulting data is presently in preparation. An overview of the Plot 2b experiment and a plan for the Plot 2b model testing efforts was provided in Hills et al. (1991). To insure that the present report is complete, much of the background material from Hills et al. (1991) is reproduced here.

2 The Las Cruces Trench Experiments: Background and Previous Work

2.1 Background

The field site is located on the New Mexico State University College Ranch, 40 km northeast of Las Cruces, New Mexico, USA. The site is on a basin slope of Mount Summerford, which is at the north end of the Dona Ana Mountains. The Dona Ana Mountains form a domal uplift complex of the younger rhyolitic and the older andesitic volcanics intruded by monzonite (Gile, Hawley and Crossman, 1970). The sediments on the mid-piedmont have young soils (6500 to 4000 years B.C.) of the Dona Ana and Onite series (coarse-loamy Typic Haplargids). Sediments on the lower-piedmont slopes are older soils (mid-late Pleistocene) dominated by the Berino series (fine-loamy Typic Haplargids). The geologic features, geomorphic surfaces, soil series, and vegetation types found in and around the field test area are typical of many areas of southern New Mexico and are similar to other arid and semiarid areas of the southwestern United States.

The climate in the region is characterized by an abundance of sunshine, low relative humidity, and an average Class A pan evaporation of 239 cm/yr. Average annual precipitation is 23 cm with 52% of the rainfall occurring between July 1 and September 30. The average monthly maximum air temperature is highest in June at 36 C and lowest in January at 13 C.

To provide site characterization data and to provide horizontal access to the experimental plots, a trench was dug in the undisturbed soil at the site. After excavation, 9 soil layers were identified (Wierenga et al., 1989a) based on the observed morphological horizons on the west wall of the trench and on the hydraulic properties of each layer. These 9 layers are shown as different shades in Figure 2.1. The upper most layer (0.00 to 0.15 m depth) shows some organic matter accumulation and some evidence of clay eluviation. There are many roots in this layer. The soil is not effervescent and its structure is massive. The soils of the deeper layers range from slightly to strongly effervescent and possess a subangular blocky structure. The average bulk density for the 9 layers range from 1.66 to 1.74 g/cm³. Average CaCO₃ content ranges from 1.4% in the top layer to 22.6% in the eighth layer. The average coarse fraction ranges from 19.5% in layer 3 to 34.6% in layer 9. The results of the particle size analysis of the 50 soil samples taken from each layer indicate that the soils are sands, sandy loams, loamy sands, and sandy clay loams. Layers 2, 3, 4, 6, 8, and 9 show evidence of carbonate accumulation. There are various buried arroyos visible

along the trench walls. The soil in these buried arroyos have no structure and the texture is gravelly sandy loam.

2.2 Experiments

The overall goals of the Las Cruces Trench experiments were to provide data to test stochastic and deterministic models for water flow and transport in spatially variable, unsaturated soils and to examine site characterization methods for very dry sites. To meet the goal of model testing, the Las Cruces Trench experiments were designed with the following objectives in mind:

- The hydraulic properties for the site should be characterized in sufficient detail so that the site can be modeled using deterministic and stochastic models.
- The boundary conditions on water flow and solute transport should be carefully controlled to minimize ambiguities associated with model testing.
- The movement of water and solute through the soil profile during infiltration and during redistribution should be monitored in sufficient detail so that the effect of spatial variability can be defined.

To accomplish these goals, two types of experiments were performed. The first type were *in situ* and laboratory based experiments designed to characterize the site. The second type were dynamic experiments designed to observe water and solute transport in a heterogeneous soil. A summary of the parameters measured during these experiments is given in Table 2.1.

2.2.1 Characterization Experiments

To characterize the hydraulic properties of the site, a trench 26.5 m long, 4.8 m wide and 6.0 m deep was dug in undisturbed soil. The walls of the trench were excavated vertically and reinforced to prevent cave-in. The trench and adjacent irrigated areas have been covered to prevent surface runoff and recharge due to rainfall and to minimize evaporation. A total of 50 undisturbed core samples and 50 disturbed soil samples were taken along the north wall of the trench at 0.5 m intervals (in the horizontal direction) from the nine different soil layers. The sampling depths within each layer are denoted by the circles in Figure 2.1. To provide data to determine the vertical correlation length,

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Figure 2.1. Soil Morphology at the Las Cruces Trench Site

Table 2.1. Parameters Measured During the Las Cruces Trench Experiments

Parameter	Scale	Technique	Reference
Characterization Variables			
K_{sat}	8 cm	Measured flow through saturated cores	Elrick et al. (1980), Wierenga et al. (1989a)
K_{sat}	10 cm	Borehole permeameter	Reynolds et al. (1984), Wierenga et al. (1989a)
θ_r , θ_s , α , n	8 cm	Cores and constant pressure apparatus combined with parameter estimation	Wierenga et al. (1989a)
Particle size distribution	8 cm	Soil sieves and modified pipet method	Gee and Bauder (1986), Wierenga et al. (1989a)
Dynamic Variables			
θ	50 cm	Neutron Probe	Wierenga et al. (1990)
h	2 cm	Tensiometer	Wierenga et al. (1990)
Concentration of tracers	2 cm	Solute samplers and soil sampling	Wierenga et al. (1990)

cores and disturbed soil samples were also taken at approximately 13 cm depth intervals to a depth of slightly over 6 m in the vertical direction at three locations along the length of the trench. Altogether, a total of 594 soil cores and 594 disturbed soil samples were taken to the laboratory for the estimation of their bulk density, saturated hydraulic conductivity and the soil-water retention curve.

The saturated hydraulic conductivity of the soil was determined *in situ* with the Guelph permeameter method (Reynolds et al., 1984). Vertical holes, 10 cm in diameter by 15 cm deep, were drilled into the undisturbed soil adjacent to each location where core samples were taken (50 per soil layer spaced 0.5 m apart for each of the 9 soil layers) along the north trench wall. Using the Guelph permeameter, a constant water level was maintained in each hole and the water outflow rate measured. The resulting *in situ* values for K_{sat} ranged from 9.3 to 13000 cm/day with the mean $\ln(K_{sat})$ of 6.024 (i.e., $K_{sat}=413.2$ cm/day) and a standard deviation on $\ln(K_{sat})$ of 1.21 (Hills and Wierenga, 1991). The saturated hydraulic conductivity of each core was also measured by applying a constant head differential

across the cores and measuring the outflow using the method of Elrick et al. (1980). The corresponding laboratory values for K_{sat} ranged from 1.4 to 6731 cm/day with the mean $\ln(K_{sat})$ of 5.5988 (i.e., $K_{sat}=270.1$ cm/day) and a standard deviation on $\ln(K_{sat})$ of 1.32 (Hills and Wierenga, 1991). The wet range of the soil water retention curves was determined by placing the saturated cores from each location into pressure boxes, subjecting them to differential pressures ranging from 10 to 300 cm H₂O, and measuring the total outflow at each differential pressure. Once outflow ceased at 300 cm H₂O pressure, the cores were oven dried and the bulk density and water contents determined. The disturbed soil samples from each location were sieved, air-dried, and used with a standard pressure plate apparatus (Soil Moisture Equipment Co., Santa Barbara, CA) to determine soil-water retention data in the dry (1 to 15 bar) range.

The NLIN procedure of SAS (SAS Institute Inc., 1985) was used to find least-squares estimates of the parameters α and n in the van Genuchten (1980a) water retention model for each core location. This model is given by

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$$S_e = \frac{\theta - \theta_r}{\theta_s - \theta_r} = \frac{1}{[1 + (\alpha|h|)^n]^m} \quad (2.1)$$

$$m = 1 - \frac{1}{n} \quad (2.2)$$

where θ , θ_r and θ_s are the volumetric water content, residual water content, and saturated volumetric water content, α and n are parameters that define the shape of the curves, and h is pressure head. The residual water content θ_r was set to the measured 15 bar water content value and θ_s was set to the gravimetrically determined value for each sample location. Given estimates of the parameters in Eq. (2.1) and laboratory estimates of the saturated conductivity, K_{sat} , at each location, Mualem's model (Mualem, 1976), as developed by van Genuchten (1980a) for Eq. (2.1), can be used to predict the unsaturated hydraulic conductivity as a function of water content for each location.

$$K = K_{sat} S_e^{1/2} \left[1 - (1 - S_e^{1/m})^m \right]^2 \quad (2.3)$$

In addition to estimating the parameters that appear in Eqs. (2.1) and (2.3) for each core sample, estimates for the hydraulic parameters were obtained for a uniform soil model and for a layered soil model. The layers in the layered soil model correspond to the 9 soil layers identified at the site. The saturated hydraulic conductivity for each soil layer was estimated by taking the geometric mean of the 50 laboratory measured saturated hydraulic conductivities obtained from each soil layer. Likewise, the water retention data from all 50 samples from a given layer were used to estimate α , n , θ_r , and θ_s for a single water retention curve for that layer. For the uniform soil model, the geometric mean of 450 laboratory measured saturated hydraulic conductivities (9 layers with 50 per layer) was used to estimate a uniform soil saturated hydraulic conductivity value. Likewise, the water retention data for all 450 sample locations were simultaneously used to estimate single values for each of the parameters α , n , θ_r , and θ_s in a least-squares sense. This resulted in a single water retention curve (i.e. uniform soil model) for the entire site.

Detailed information on the site characterization experiments, the parameter estimation procedures, and the experimental results are provided in Wierenga et al. (1989a).

2.2.2 Dynamic Experiments Performed during Phase I

As part of the Phase I INTRAVAL model testing effort, two dynamic field experiments were performed. A third experiment was performed as part of Phase II and is discussed in a following chapter. During the first experiment (denoted the Plot 1 experiment), water containing tritium was applied at a rate of 1.82 cm/day for 10 days on an area immediately adjacent to the south trench wall. Water without tritium was applied at the same rate for an additional 76 days. During the second experiment (denoted the Plot 2a experiment), water containing tritium and bromide was applied at a rate of 0.43 cm/day for 11.5 days on an area immediately adjacent to the north trench wall. Water application continued at the same rate without tracers for an additional 64 days. A plan view of the trench and the irrigated areas is shown in Figure 2.2. The movement of water was monitored during infiltration and redistribution for both experiments. Tracer movement was monitored during infiltration for the Plot 1 experiment and during both infiltration and redistribution for the Plot 2a experiment.

To monitor water content changes during the experiments, neutron probe access tubes were installed in several vertical planes extending through the irrigated area (see Figure 2.2). The access tubes were used to take water content measurements at 0.25 m increments down to 6 m. A total of 18 tubes were installed in Plot 1 and 43 tubes for Plot 2. An additional 5 tubes were installed to a depth of 1.5 m in Plot 1. An array of tensiometers was installed on the trench walls adjacent to each experimental plot. The tensiometers were installed at a slight incline 0.5 m into the soil formation. A total of 79 tensiometers were installed for the Plot 1 experiment and 49 tensiometers for the Plot 2a experiment. Two arrays of solute samplers were also installed through the trench walls for the Plot 1 and 2a experiments (one each). A total of 24 solute samplers were installed for the Plot 1 experiment and 49 samplers for the Plot 2a experiment. Nine of the tensiometers from the Plot 2a experiment were converted to solute samplers after the wetting front had passed. Additional tensiometers and solute samplers were installed prior to the start of the Plot 2b experiment. The tensiometers and solute samplers for the Plot 2b experiment are shown in Figure 2.3.

Detailed information on the Plot 1 and 2a experiments as well as experimental results is provided in Wierenga et al. (1990).

A suite of additional experiments have been performed using laboratory soil columns and 6 m deep field lysimeters. The large lysimeter tests (described in Wierenga

Figure 2.2. Plan View for the Las Cruces Trench Experiments

Background

Figure 2.3. Tensiometers and Solute Samplers for the Plot 2a and 2b Experiment

et al., 1986; Wierenga and van Genuchten, 1989a; and Hills et al., 1989b) as well as the laboratory column tests were used to estimate transport parameters (i.e., Peclet numbers, dispersion coefficients, etc.) that are useful to understand field transport in soils of similar physical and chemical characteristics. These experiments consist of infiltration and redistribution tests in uniform and layered soils under similar flow conditions as those imposed in the field tests.

2.3 Modeling Performed During Phase I of INTRAVAL

The soil at the Las Cruces Trench Site was conceptualized to be a spatially variable, coarse grained, porous medium. Since the experiments were conducted with irrigation rates much smaller than the saturated hydraulic conductivities characteristic of the site, the porous medium was conceptualized to be unsaturated. The Plot 1 wetting front, which was visible on the south trench wall during the infiltration phase of the experiment, showed no evidence of preferential flow. Preferential flow induced by cracks, roots, and fractures was thought to be insignificant during this experiment due to the lack of visual evidence of preferential flow on the trench wall and due to the highly unsaturated conditions.

2.3.1 Process Models used for the Phase I Las Cruces Experiments

The process models used during Phase I of INTRAVAL for the Plot 1 and 2a experiments include the models characterizing the soil hydraulic properties and the dynamic models that are used to simulate water flow and transport. The various water flow and transport models that were used were based on Richards' equation and the convective-dispersion equation. The differences in the models lie largely in their incorporation of deterministic or stochastic models for spatial variability of the soil hydraulic properties.

Water retention was modeled by van Genuchten's relationship with the Mualem-van Genuchten model (van Genuchten, 1989a) generally used for the unsaturated hydraulic conductivity. These models are given by Eqs. (2.1) and (2.3).

Richards' equation was used to model water flow through the unsaturated porous media. This equation can be written in tensor notation as

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial x_i} \left[K_{ij} \left(-\frac{\partial h}{\partial x_j} + \frac{\partial z}{\partial x_j} \right) \right] \quad (2.4)$$

where K_{ij} is the hydraulic conductivity tensor, z the elevation above a reference datum, $x_i, i=1,2,3$ are the coordinates, and t is time.

Several different models were used for the spatial variability of K_{ij} and for the water retention characteristics. The models ranged from simple uniform, isotropic soil models to a pressure head dependent, anisotropic, unsaturated, hydraulic conductivity expression which are based on stochastic theory. In several cases, stochastic realizations of the property fields were used.

The advective-dispersive equation was used to model solute transport. This equation is given by

$$\frac{\partial}{\partial t} (R\theta c) = \frac{\partial}{\partial x_i} \left(\theta D_s \frac{\partial c}{\partial x_i} - q_i c \right) \quad (2.5)$$

where R is the retardation factor, D_s is the dispersion coefficient, and q_i are the Darcian fluxes along the x_i directions. In the models used here, D_s was assumed to be a scalar. The dispersion coefficient is given by

$$\theta D_s = \theta D_m + \epsilon |q| \quad (2.6)$$

where D_m is the molecular dispersion coefficient, ϵ is the dispersivity, and q is the magnitude of the Darcian flux.

The geometry of the irrigation system (see Figure 2.2) was such that the flow could be modeled deterministically as two-dimensional over much of the experimental region. When two-dimensional models were used, the three-dimensionality of the actual flow due to spatial variability was either ignored or modeled through effective media approximations. One model, which synthesized conditions analogous to the Las Cruces Trench Experiments, used a single three-dimensional realization of a stochastic hydraulic property model. The resulting Richards' equation was solved in three dimensions.

2.3.2 Summary of Modeling Efforts during Phase I of INTRAVAL

Early modeling of the Las Cruces Trench site using the field data sets are described in MIT reports (thesis, etc.), in

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Hills et al. (1989a, 1989b), and in Wierenga et al. (1990). More recently, scientists from the Center For Nuclear Waste Regulatory Analysis at the Southwest Research Institute; HydroGeoLogic, Inc.; KEMAKTA Consultants Co.; Massachusetts Institute of Technology; New Mexico State University; Pacific Northwest Laboratory; and Sandia National Laboratories have used the Las Cruces data to test transient models for water flow and solute transport through unsaturated soils. These models range from two-dimensional deterministic simulations of water flow and transport through uniform isotropic soils to three-dimensional simulations of water flow through fully heterogeneous, anisotropic soils. Stochastic models include one- and two-dimensional simulations of water flow using Monte-Carlo methods and two-dimensional simulations of water flow using the techniques of Mantoglou and Gelhar (1987a, b, c). Descriptions of the various models and model results are provided in the INTRAVAL Phase I Final Report on the unsaturated zone test cases (Voss and Nicholson, 1993). A summary of the modeling efforts is presented in Table 2.2. Brief descriptions of the features of these models as applied to the Las Cruces Trench Site follow.

The Center for Nuclear Waste Regulatory Analysis

The Center for Nuclear Waste Regulatory Analysis modeled water flow using BIGFLO (Ababou, 1988; Ababou and Gelhar, 1988; Voss and Nicholson, 1993). BIGFLO is a transient, three-dimensional, finite difference simulator for saturated or partially saturated flow in a fully heterogeneous porous media. Over 300,000 finite-difference cells were used to represent soil heterogeneity. A single van Genuchten function was used for the moisture retention curve. A stochastic exponential model ($K = K_{sat} \exp(\alpha h)$) was assumed for the unsaturated conductivity. The parameters K_{sat} and α defining this model were assumed to be spatially correlated replicates of two log-normally distributed, three-dimensional, independent random fields. The three-dimensional correlation structures of these fields were taken to be anisotropic. Data collected at the trench were used to infer hydraulic properties and their statistics. Water flow for the Plot 1 experiment was modeled during infiltration and drainage for conditions somewhat analogous but not directly comparable to those that occurred at the site.

HydroGeoLogic, Inc.

HydroGeoLogic used VAM2D to simulate water flow and tritium transport for the Plot 2a experiment at the Las Cruces Trench Site (Huyakorn et al., 1989; Voss and Nicholson, 1993). VAM2D is a transient, two-dimensional,

finite element code that models Richards' equation and the convective-dispersion equation. Several models for the spatial variability of the soil hydraulic properties of the Las Cruces Trench Site were evaluated. These include 1) a uniform, isotropic soil model with hydraulic properties of a typical sandy loam soil; 2) a uniform, isotropic soil model with hydraulic properties obtained from the Las Cruces characterization data; 3) a uniform soil model with an anisotropic saturated hydraulic conductivity; 4) a non uniform, isotropic soil model with spatial variation of hydraulic properties based on the spatial variation measured at the Las Cruces Trench Site; and 5) a uniform, anisotropic soil model with a pressure head dependent, anisotropic, hydraulic conductivity based on the stochastic arguments of Yeh et al. (1985a, b, c).

KEMAKTA Consultants Co.

KEMAKTA used TRUST+TRUMP to model water flow and solute transport for the Plot 2a experiment (Collin and Rasmuson, 1990; Voss and Nicholson, 1993). The codes are based on integrated finite difference algorithms which model Richards' equation for an unsaturated porous media and the convective-dispersive equation. Several models for the soil properties were considered. These are 1) a homogeneous, isotropic soil model based on the uniform van Genuchten parameters provided in the Las Cruces Database (see Wierenga et al., 1989a, 1990 for a discussion of the database); 2) a homogeneous soil model with modified water retention and unsaturated hydraulic conductivity curves that allow the dry initial conditions to be better modeled; 3) a layered soil model based on the layered soil van Genuchten parameters provided in the Las Cruces Database.

Massachusetts Institute of Technology

Water flow for the Plot 1 experiment was modeled by the Massachusetts Institute of Technology using a stochastic model and the results were compared to those of a simpler deterministic model (Voss and Nicholson, 1993). The stochastic model uses an effective mass balance equation which incorporates effective soil parameters assuming a statistically uniform equivalent media (Gelhar, 1984; Mantoglou et al., 1987a,b,c; Polmann et al., 1988; Yeh et al., 1985a,b,c). A finite element algorithm with modified Picard iteration was used to solve the transient mass balance equation for water flow in two dimensions. The soil is assumed to be isotropic and homogeneous on the local scale; to behave as a stationary stochastic process on the large scale; and to possess a log-normally distributed unsaturated hydraulic conductivity, a normally distributed local water content, and a normally distributed local

tension. Comparisons were made between the water flow predictions of the stochastic model and a simpler deterministic model. The parameters used were based on data obtained from the Las Cruces Trench site and on Maddock soil unsaturated conductivities obtained from another site (the unsaturated conductivities for the Las Cruces Trench site were not available at that time).

New Mexico State University

New Mexico State University used a transient, two-dimensional, water content based, finite difference model for Richards' equation to simulate infiltration and redistribution for the Plot 2a experiment (Hills et al., 1989a; Kirkland et al., 1992; Voss and Nicholson, 1993). A transient, two-dimensional finite difference algorithm for the convective-dispersion equation was used to model solute transport. The simulations assumed a uniform, isotropic soil using the van Genuchten parameters provided in the Las Cruces database.

Pacific Northwest Laboratory

Several codes were used by Pacific Northwest Laboratory to model water flow for the Plot 1 experiment (Voss and Nicholson, 1993). These were UNSAT-H and UNSAT2 (Fayer et al., 1986; Davis and Neuman, 1983), which are one- and two-dimensional finite element codes which solve Richards' equation, and TRACER3D (Travis, 1984), which is a finite difference code for Richards' equation and the convective-dispersive equation. The codes were used to simulate transient one- and two-dimensional water flow

during infiltration using 1) a homogeneous, isotropic soil model, 2) a three layer soil model, and 3) a three layer soil model with a high conductivity zone in the third layer. Transport was not simulated by PNL. The soil property models were based on preliminary characterization data obtained from the Las Cruces Trench Site. In addition, the finite difference code PORFLO-3 was used to simulate two-dimensional water flow and solute transport for the Plot 2a experiment (Rockhold and Wurstner, 1991). Three simulation cases were considered. In the first case, the soil was assumed to be uniform with homogeneous, isotropic hydraulic and transport properties. The remaining cases utilized single stochastic realizations of randomly heterogeneous hydraulic conductivity fields generated from the cumulative probability distribution of the measured data.

Sandia National Laboratories

Sandia National Laboratories modeled water flow for the Plot 1 and Plot 2a experiments using a one-dimensional infiltration model and using the two-dimensional Richards equation code VAM2D (Huyakorn et al., 1989; Voss and Nicholson, 1993). VAM2D is a transient, two-dimensional, finite element based code that models Richards' equation and the convective-dispersion equation. The soil was assumed to be homogeneous and isotropic and the water flow and transport were assumed to be transient and two-dimensional during each realization. Soil properties for each realization were based on individual samples taken from the population of core samples analyzed during the Las Cruces characterization experiments.

Background

Table 2.2. Previous Modeling of the Las Cruces Trench Experiments

Group	Model	Comments
CNWRA	BIGFLOW	Finite difference code for high resolution water flow simulations. Modeled a 3-D, randomly heterogeneous and stratified soil with boundary conditions similar to Plot 1 but with wetter initial conditions.
HGL	VAM2D	Finite element code for water flow and transport. Modeled Plot 2a with several levels of heterogeneities (isotropic and anisotropic) in 2-D.
KCC	TRUST +TRUMP	Integrated finite difference code for water flow and transport. Modeled Plot 2a as a homogeneous and a layered soil in 2-D.
MIT		Finite element code for water flow using modified Picard Iteration. Modeled Plot 1 using 3-D effective media stochastic property models in a 2-D simulation.
NMSU		Water Content based finite difference code for water flow and transport. Modeled Plot 2a as a homogenous soil in 2-D.
PNL	UNSAT-H UNSAT2	One and two-dimensional finite element codes for water flow. Modeled Plot 1 water flow with several levels of heterogeneities in 2-D.
	TRACER3D PORFLO-3	Finite difference codes for water flow and transport. Modeled Plot 1 and 2a water flow and transport with several levels of heterogeneities in 2-D including several realizations of randomly heterogeneous hydraulic conductivity fields.
SNL	VAM2D	Finite element code for water flow and transport. Monte-Carlo simulation of 2-D water flow using VAM2D with multiple realizations of a uniform soil model. Analytic 1-D models are used.

CNWRA - Center for Nuclear Waste Regulatory Analysis

HGL - HydroGeologic, Inc.

KCC - KEMAKTA Consultants Co.

MIT - Massachusetts Institute of Technology

NMSU - New Mexico State University

PNL - Pacific Northwest Laboratory

SNL - Sandia National Laboratories

3 The INTRAVAL Phase II Model Testing Experiment

As part of the Phase I INTRAVAL model testing effort, seven organizations modeled the first, the second, or both experiments. These experiments were not blind in the sense that most of the modelers had access to the dynamic experimental data prior to their modeling efforts. This allowed the modelers to present comparisons between model predictions and experimental observations but also provided the opportunity for model calibration. These comparisons were generally qualitative (visual comparisons of contour plots of water contents and solute concentrations) rather than quantitative and no direct comparisons were made between the model predictions performed by the different modeling organizations.

3.1 The Plot 2b Experiment

To provide a more complete data set, especially with regard to solutes, a third experiment (denoted the Plot 2b experiment) was performed. The Plot 2b experiment used the same irrigation system (see Figure 2.2) as the Plot 2a experiment. Additional tensiometers, solute samplers, and neutron probe access tubes were installed. Different water application rates and different initial conditions were used during the Plot 2b experiment to test the ability of models to predict water flow and solute transport given model calibration data obtained under these different conditions. A summary of the application history of water and solute during the Plot 2b experiment is shown in Figure 3.1. The irrigated area was 1.22 by 12 meters with an average water application rate of 1.82 during the 70 day irrigation period. Tritium, bromide, boron, chromium, and the organic compounds pentafluorobenzoic acid (PFBA) and 2,6-difluorobenzoic acid (DFBA) were applied with the irrigation water during the Plot 2b experiment. Chromium, boron, and PFBA were applied during the first 15 days of irrigation with tritium, bromide, and DFBA applied during days 29 through 44 of irrigation. The actual application history for the Plot 2b experiment, including concentrations, is available in the Las Cruces Database. The water application rate was approximately 4 times larger than that used during the Plot 2a experiment. In addition, the initial water content in the upper half of the monitored soil profile was significantly wetter due to the water applied during the Plot 2a experiment. As a result of the increase in water application rate, the water and solute moved to a greater depth during the Plot 2b experiment than during the Plot 2a experiment. All concentrations of tritium and bromide that appear in the Las Cruces Database for the Plot 2a and 2b experiments are relative to the concentrations applied during the Plot 2a experiment. Since the concentration of tritium applied during the Plot 2b

experiment was 0.622 of that applied during the Plot 2a experiment, the modelers used a value of 0.622 for the applied concentration of tritium for the Plot 2b experiment. Both blind and non-blind model predictions were provided to NMSU for model testing. Blind predictions are defined to be those predictions that were made before the modeler had access to or had seen the results of the Plot 2b experiment. After the blind predictions were submitted to NMSU, quantitative comparisons were made by NMSU and reported at an INTRAVAL meeting. Additional predictions (denoted as not blind) were submitted to NMSU after the experimental results were reported.

3.2 Available Calibration Data

While the Plot 2b experimental data was not provided to the modelers until blind model predictions were provided to NMSU, the data from the characterization experiments and from the Plot 1 and 2a experiments were available. These data were available in both raw and processed form. The raw data included water retention data, density profiles, particle-size analysis data, and saturated hydraulic conductivities measured through both laboratory and *in situ* techniques during the characterization experiments; and water content data, tensiometer data, solute concentrations, and water applications rates measured during the Plot 1 and Plot 2a experiments. In addition, morphological mapping of the trench face, drip irrigation distribution tests, and outflow and inflow measurements from large and small column tests using similar soils were on file at NMSU and at UA.

The processed data are reported in Wierenga et al. (1986, 1989a, 1990). These data consist of moisture profiles determined from neutron probe calibration curves; tension profiles from tensiometer data mapped as a function of time; tritium profiles and breakthrough curves (obtained from solute sample analysis); and wetting front observations from the first trench experiment obtained by visual mapping the wetting front advance with time. In addition, the van Genuchten water retention parameters α and n for each of the 594 core sample locations and the parameters for uniform and layered soil models were estimated and are discussed in Wierenga et al. (1989a) and reproduced in Table 3.1. The parameters listed in Table 3.1 are based on 450 of the sample locations which were taken from a 9 deep by 50 wide grid spaced over a 6 m deep by 25 m wide area along the north trench face. The remaining samples were taken from 3 vertical transects along the north trench face and are discussed in Wierenga et al.

Phase II

Figure 3.1. The Plot 2b Experiment

Table 3.1. van Genuchten Parameters for the Las Cruces Test Site. Data based on core samples taken during excavation of the trench.

Layer	Depth, cm	θ_s	θ_r	α 1/cm	n	K_{sat} cm/day
1	0 to 15	0.3483	0.0949	0.04194	1.9026	539.2
2	15 to 140	0.3434	0.0914	0.06237	1.5278	250.0
3	140 to 205	0.3359	0.0849	0.05960	1.5742	266.9
4	205 to 250	0.3129	0.0714	0.06772	1.5373	299.8
5	250 to 305	0.3021	0.0716	0.04039	1.5496	250.0
6	305 to 370	0.2942	0.0896	0.07029	1.7117	334.0
7	370 to 460	0.3104	0.0726	0.02719	1.4177	220.6
8	460 to 540	0.3248	0.0834	0.04110	1.3826	171.5
9	540 to 600	0.3061	0.0778	0.04679	1.4315	225.9
all	0 to 600	0.3209	0.0828	0.05501	1.5093	270.1

(1989a). The saturated hydraulic conductivities listed in Table 3.1 are based on core samples rather than on the *in situ* experiments performed at the site (Wierenga et al., 1989a).

Tritium, chromium, pentafluorobenzoic acid (PFBA), and 2,6-difluorobenzoic acid (DFBA) were applied during the Plot 2b experiment. Porro (1989) and Porro and Wierenga (1992) have performed a series of laboratory and field column studies to help characterize the transport parameters of tritium, bromide, chromium, boron, and chloride for soils taken from the Las Cruces Trench site. Column studies utilizing PFBA and DFBA have not been performed using soils from the site, but PFBA and DFBA are non-reactive anions and are thus expected to possess the same transport parameters as bromide.

In one of the column studies performed by Porro (1989) and Porro and Wierenga (1993), a field scale vertical column (95 cm diameter by 610 cm long) was filled with Berino loamy fine sand (Fine-loamy, mixed, thermic, Typic Haplargid) obtained from a location near the trench site. Water was applied at a rate of 1.84 cm/day to the top of the column through drip irrigators and removed from the bottom through suction candles so that unsaturated conditions were maintained. Tracer pulses were applied with the water after steady flow conditions were reached and break-through data were obtained from solute samples taken at six depths in the column. The multiparameter optimization program (CXTFIT) of Parker and van Genuchten (1984) was used to estimate transport parameters utilizing the following equation (parameters in other forms of the transport equation were also estimated by Porro and Wierenga but not reported here):

$$R \frac{\partial c}{\partial t} = D_s \frac{\partial^2 c}{\partial x^2} - v \frac{\partial c}{\partial x} - Kc \quad (3.1)$$

where R is the retardation factor, c is concentration, t is time, D_s is the dispersion coefficient, x is depth below the surface, v is the average pore water velocity, and K is the first-order kinetic rate coefficient.

A set of transport parameters was estimated for each depth using only the data from that depth. The tritiated water was assumed to move exactly as unlabeled water. The retardation factor R of tritium was thus assumed to be 1.0. The observed movement of the tritium through the soil profile was used to define the average pore water velocity to each depth. These velocities are listed in Table 3.2. The retardation factor and the dispersion coefficient were estimated for bromide while only the dispersion coefficient was estimated for tritium. The kinetic rate coefficients K were taken to be zero for tritium and bromide. The retardation factor, the dispersion coefficient, and the first-order kinetic rate coefficient were also estimated for chromium. The resulting parameter estimates are shown in Table 3.2 along with the corresponding r^2 values.

The dispersivity ϵ is related to the dispersion coefficient through the following equation:

$$D = D_m + \epsilon v \quad (3.2)$$

where the molecular diffusion coefficient D_m is often taken to be 1.0 cm²/day. Given the estimates for D and v , the dispersivity ϵ can be calculated from the above equation. The resulting values are shown in Table 3.2. Porro and Wierenga (1992) report slightly different values for the

Table 3.2. Transport Parameters for the Uniform Soil Field Column: The water application rate was 1.84 cm/day.

Depth, cm	ν , cm/d	R	D , cm ² /day	ϵ , cm	K , 1/d	r^2
Tritium						
82	18.37	1.00	40.45	2.15	0.0	1.00
125	16.51	1.00	66.08	3.94	0.0	0.99
220	17.14	1.00	52.50	3.00	0.0	0.92
310	13.21	1.00	67.25	5.02	0.0	0.99
400	10.85	1.00	84.59	7.70	0.0	0.96
500	12.29	1.00	61.91	4.96	0.0	0.97
Bromide						
82	18.37	0.87	21.64	1.12	0.0	0.99
125	16.51	0.85	34.41	2.02	0.0	0.99
220	17.14	0.82	16.87	0.93	0.0	1.00
310	13.21	0.80	51.24	3.80	0.0	0.98
400	10.85	0.82	40.07	3.60	0.0	0.97
500	12.29	0.84	34.36	2.71	0.0	0.98
Chromium						
82	8.37	1.06	26.56	1.39	0.033	0.99
125	16.51	1.01	43.19	2.56	0.029	0.99
220	17.14	1.00	24.37	1.36	0.026	0.98
310	13.21	0.99	42.22	3.12	0.020	0.96
400	10.85	1.00	23.09	2.04	0.033	0.97
500	12.29	1.02	18.48	1.42	0.032	0.97

dispersivity since they assumed that $D = \epsilon \nu$ which neglects the effect of molecular diffusion.

3.3 Independence Between Data Sets

The hydraulic characterization data were estimated from *in situ* experiments and core samples taken from an area adjacent to the Plot 1, 2a, and 2b infiltration and redistribution experiments. The results from the Plot 1 and 2 experiments were not used to calibrate or redefine the characterization data in any way. The characterization data are thus independent of the Plot 1 and 2 data. The Plot 1 and Plot 2a data were taken from opposite sides of the trench and at different flow rates and are thus independent.

The neutron probe data, the tensiometer data, and the solute samples taken through the trench wall during the Plot 2b experiment are taken from the same locations as during the Plot 2a experiment. However, additional solution samplers and neutron access tubes were installed as the water and solute fronts moved through the soil profile. The Plot 2a and 2b experiments were at different flow rates and the Plot 2b experiment uses additional tracers (boron, chromium, pentafluorobenzoic acid, and 2,6-difluorobenzoic acid) as well as tritium and bromide. The initial water content

profile prior to the start of the Plot 2b experiment was considerably wetter than the profile at the start of the Plot 2a experiment. In contrast to the Plot 2a experiment, non zero initial conditions on tritium and bromide were present during the Plot 2b experiment. In addition, the depths reached by the water and solute were approximately twice those obtained during the Plot 2a experiment. Thus, the Plot 2b data is independent of the Plot 2a data in the sense that different boundary and initial conditions were used but dependent in the sense that the experiments were run at the same location using expanded versions of the same monitoring systems.

Additional core samples were taken for chemical analysis during and after the Plot 2b experiment from locations not previously sampled. This data is thus independent of the solute concentration data obtained through the trench face during the Plot 2a and 2b experiments.

3.4 Spatial and Temporal Scales

Due to the variety of characterization and dynamic experiments performed and due to the duration of the experiments, the spatial and temporal scales range over several orders of magnitude. Temporal scales include sampling times for infiltration events ranging from hours

(during early infiltration) to years for later observations. The time period utilized for the Plot 1, 2a and 2b infiltration tests exceeded 70 days (i.e. the irrigation period) with measurements taken every several days. During redistribution, the Plot 1 and 2a experiments were monitored over several years and the Plot 2b experiment was monitored for a year and a half. During the early phases of redistribution, the dynamic variables were monitored every several days with the monitoring interval increasing to months during the later phases of redistribution.

The number of monitoring locations for tensions exceeded 50 during the Plot 2a experiment and 100 during the Plot 2b experiment. The number of monitoring locations for solute in the trench face also exceeded 50 during the Plot 2a experiment and 85 during the Plot 2b experiment. Over 1000 neutron probe monitoring locations were used to measure water content during each of the Plot 2a and 2b experiments. The spatial scales of the experiments range from several cm (core and disturbed soil samples) to several tens of meters (field experiments). Spatial scales for the soil heterogeneities range from less than a meter to several meters. Based on approximately 450 *in situ* and laboratory measurements, the saturated hydraulic conductivity ranged over three orders of magnitude. The van Genuchten water retention parameters α and n range over three and one orders of magnitude, respectively. There appear to be no complex discontinuities in the 6 m soil profile such as faults or fracture networks.

3.5 Biases Inherent in the Data

There are several sources for bias in the data. These are listed below:

1. The soil water retention characteristics determined in the laboratory may not be a true representation of the water release characteristics in the field. The core samples may not accurately represent *in situ* conditions since the cores may have been disturbed some-what during the sampling process. Also, sampling and measurement techniques have not been developed to the point that the entire (wet to dry) range of the water retention curve can be measured by a single instrument. Pressure plate techniques may tend to over estimate water contents at high tensions. Hence field observations should be used to supplement laboratory measurements when possible.
2. Since tensiometers only operate in the wet range, the majority of the tension data will be in a range where tensions are not too large (<150 cm H₂O). This will tend to bias the tensiometer readings toward wetter environments than are normally experienced in arid regions.
3. In contrast, neutron probes can measure very small water contents but the effective area of the measurement is large. The effective area is largely a function of water content and can range up to 0.5 m in diameter. As a result, neutron probes are inherently poor at defining sharp wetting fronts. In addition, the magnitude in the observed spatial variability in water content will be smaller than the true value due to the spatial averaging effect of the measurement. Thus caution must be exercised when comparing predictions of point values of water content to observations.
4. The unsaturated conductivity functions determined from pore-size models may inadequately describe the actual unsaturated conductivity values in the field.
5. Solute concentration cannot be accurately measured if sufficient water is not present in the soil to obtain sufficient sample through the solute samplers. Thus the concentrations that are successfully measured are biased toward the wetter locations in the soil profile.

4 The Models

Water content predictions for the Plot 2b experiment were provided by the Center for Nuclear Waste Regulatory Analysis (CNWRA), Massachusetts Institute of Technology (MIT), New Mexico State University (NMSU), Pacific Northwest Laboratory (PNL), and the Bureau of Economic Geology (BEG) at the University of Texas. Solute transport predictions were provided by New Mexico State University and Pacific Northwest Laboratory.

All models for water flow were either based on, or reduced to Richards' equation when applied to the Plot 2b experiment. Richards' equation for a heterogeneous media, for which the principal directions of the conductivity tensor are aligned along the coordinate directions, is

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial x} \left[K_x \frac{\partial h}{\partial x} \right] + \frac{\partial}{\partial y} \left[K_y \frac{\partial h}{\partial y} \right] + \frac{\partial}{\partial z} \left[K_z \left(\frac{\partial h}{\partial z} - 1 \right) \right] \quad (4.1)$$

where x is the horizontal coordinate parallel to the trench face, y is the horizontal coordinate normal to the trench face, z is the vertical coordinate measured downward, and t is time, θ is the volumetric water content, h is pressure, and K_x , K_y and K_z are the unsaturated hydraulic conductivities in the x , y and z directions, respectively. With the exception of the MIT model, the van Genuchten or modified van Genuchten models (1980a, modifications are described below) were used for the water retention and unsaturated hydraulic conductivity curves given by Eqs. (2.1) through (2.3) and repeated here for convenience.

$$S_e = \frac{\theta - \theta_r}{\theta_s - \theta_r} = \frac{1}{\left[1 + (\alpha|h|)^n \right]^{1/m}} \quad (4.2)$$

$$m = 1 - \frac{1}{n} \quad (4.3)$$

$$K = K_{sat} S_e^{1/2} \left[1 - (1 - S_e^{1/m})^m \right]^2 \quad (4.4)$$

where θ_r and θ_s are the residual and saturated volumetric water content, α and n are parameters that define the shape of the curves, and K_{sat} is the saturated hydraulic conductivity along the direction of interest.

The convection/dispersion equation used for the model predictions presented here is

$$\begin{aligned} \frac{\partial}{\partial t} (R\theta c) = & \frac{\partial}{\partial x} \left(\theta D_x \frac{\partial c}{\partial x} - q_x c \right) \\ & + \frac{\partial}{\partial y} \left(\theta D_y \frac{\partial c}{\partial y} - q_y c \right) \\ & + \frac{\partial}{\partial z} \left(\theta D_z \frac{\partial c}{\partial z} - q_z c \right) \end{aligned} \quad (4.5)$$

where R is the retardation factor, D_s is the dispersion coefficient, and q_x , q_y and q_z are the Darcian fluxes in the x , y , and z directions:

$$q_x = K_x \frac{\partial h}{\partial x} \quad (4.6a)$$

$$q_y = K_y \frac{\partial h}{\partial y} \quad (4.6b)$$

$$q_z = K_z - K_z \frac{\partial h}{\partial z} \quad (4.6c)$$

The dispersion coefficient D_s is given by

$$\theta D_s = \theta D_m + \epsilon |q| \quad (4.7)$$

where D_m is the molecular dispersion coefficient, ϵ is the dispersivity, and $|q|$ is the magnitude of the Darcian flux.

A summary of the models is provided in Table 4.1. Detailed descriptions of the models are given in the following sections. A blind model is one which was formulated before the modeler had seen the experimental results.

4.1 The Center for Nuclear Waste Regulatory Analysis

Models CNWRA1, CNWRA2, CNWRA3

The Center for Nuclear Waste Regulatory Analyses (CNWRA) submitted three models of water flow for the

Models

Table 4.1. Modeling of the Plot 2b Experiment

Group	Models	Comments
BEG	BEG1	Not Blind. Finite difference code for two phase flow and multicomponent transport. Modeled water flow in 2-D assuming uniform, isotropic soil.
CNWRA	CNWRA1	Blind. Finite volume code for water flow. Modeled water flow in 2-D using a 9 layer, isotropic soil model.
	CNWRA2	Blind. Finite volume code for water flow. Modeled water flow using a 2-D, heterogeneous 121 zone (11 x 11 grid), isotropic soil model based on trench face characterization.
	CNWRA3	Blind. Finite volume code for water flow. Modeled water flow using a 2-D, heterogeneous 3621 (51 x 71 grid), isotropic soil model based on trench face characterization.
MIT	MIT1	Blind. Finite element code for water flow using modified Picard approximation. Modeled water flow using a 3-D effective media stochastic property model (homogeneous, anisotropic) in a 2-D simulation.
NMSU	NMSU1	Not Blind. Water content based finite difference code for water flow and tritium transport. Modeled water flow and tritium transport assuming soil is homogenous and isotropic in 2-D.
	NMSU2-NMSU5	Not Blind. Water content based finite difference code for water flow and tritium transport. Modeled hydraulic properties of soil as heterogeneous, isotropic in 2-D using four property realizations sampled from the trench face characterization. Transport properties were modeled as uniform, isotropic.
PNL	PNL1	Blind. Finite difference code for two-phase flow and transport. Modeled water flow and tritium transport in 2-D using a composite van Genuchten, uniform, isotropic soil model for the hydraulic properties. Transport properties were modeled as uniform and isotropic.
	PNL2	Blind. Finite difference code for two-phase flow and transport. Modeled water flow and tritium transport assuming the hydraulic properties of the soil were uniform, anisotropic, using the modified van Genuchten parameters in the standard van Genuchten model. Transport properties were modeled as uniform and isotropic.
	PNL3	Blind. Finite difference code for two-phase flow and transport. Modeled water flow and tritium transport assuming the hydraulic properties of the soil were uniform, isotropic, and using van Genuchten parameters estimated from a 1-D inverse analysis of Plot 1 experiment. Transport properties were modeled as uniform and isotropic.
	PNL4	Blind. Finite difference code for two-phase flow and transport. Modeled water flow and tritium transport using the 2-D trench face characterization of the water retention parameters and an isotropic, 2-D heterogeneous, conditioned realization of the saturated hydraulic conductivity field. Transport properties were modeled as uniform and isotropic.

BEG - Bureau for Economic Geology, University of Texas

CNWRA - Center for Nuclear Waste Regulatory Analysis

MIT - Massachusetts Institute of Technology

NMSU - New Mexico State University

PNL - Pacific Northwest Laboratory

Plot 2b experiment. The solution domain for the models was based on a two-dimensional vertical transect aligned parallel to the trench face extending horizontally from $x=-5$ m to $x=5$ m from the center of the 1.22 meter wide strip source, and vertically to a depth of 7 m. The three models differ solely by the number of distinct rectangular parameter zones used to assign the soil hydraulic properties to the computational mesh. The least spatially complex model (CNWRA1) consisted of 9 parameter zones corresponding to the 9 distinct soil layers observed on the north face of the trench. The two more spatially complex models consisted of 121 (CNWRA2) and 3621 (CNWRA3) rectangular parameter zones defined on regular grids of 11×11 and 51×71 , respectively, in the horizontal and vertical directions. Only the $y=2$ m plane was modeled.

During earlier efforts at modeling the Plot 2a experiment, difficulties were encountered in determining a suitable set of initial pressures, since many of the initial water content values obtained from neutron probe measurements were less than the estimated residual water content of the soil. It was assumed that the soil hydraulic parameters, which were obtained from cores taken in a vertical cross-section parallel and immediately adjacent to the north face of the trench, could be directly projected normal to the north trench face and made coincident with the planar arrays of neutron probe access tubes at 2, 6 and 10 meters from the face. Any node, i , in the computational mesh that resided within the intersection of the rectangular areas of influence for soil sample location, l , and the neutron probe location, j , was assigned the pressure head

$$h_i = \frac{1}{\alpha_l} \left[\left(\frac{\theta_j - \theta_r}{\theta_s - \theta_r} \right)^{\frac{n}{1-n}} - 1 \right] \quad (4.8)$$

Although this equation is defined when $\theta_j < \theta_{rl}$, this condition implies negative saturation, and its solution is meaningless. To resolve this problem, the pressure head at any node for which this condition occurred was set to 15 bar, the pressure at which the residual water content was defined. As a result, the assigned initial water content in many portions of the model domain greatly exceeded the measured water content.

In order to eliminate the modeling errors caused by excessively wet initial conditions for the Plot 2b study, it was determined that re-estimation θ_r , α , and n was required for each of the water retention curves. Initially, a procedure suggested by Mualem (1976) was implemented whereby θ_r , α , and n are estimated subject to the constraint that the computed water retention curve passes through the point corresponding to the highest suction and lowest water

content. Rather than use the quasi-analytical procedure suggested by Mualem a similar procedure was implemented via constrained nonlinear least squares. A simple FORTRAN program was coded that called the IMSL (1987) routine, DNCONF, to determine the values of θ_r , α , and n which minimized the sum of squared differences between measured and computed water contents subject to the constraint given by

$$\theta_{\min} = \theta_r + \frac{\theta_s - \theta_r}{\left[1 + (\alpha h_{\min})^n \right]^m} \quad (4.9)$$

where m is given by Eq. (4.3).

Unfortunately there remained some locations in the model domain where the re-estimated residual water content exceeded the measured initial water content. This problem was finally resolved by adding an additional data point to each water retention curve that consisted of the lowest water content measured by the neutron probe and the highest suction measured by the thermocouple psychrometer anywhere within the experimental domain, followed by re-estimation of θ_r , α , and n .

For the 9 layer model, the van Genuchten parameters for each layer were determined using the estimation procedure described above applied to all the water retention data from cores taken within the corresponding soil horizon. The saturated hydraulic conductivities for each zone were computed by taking the geometric mean of the saturated hydraulic conductivities measured *in situ* within each layer by a Guelph permeameter. For the 121 and 3621 zone models, punctual kriging was used to estimate the soil hydraulic parameters at the center of each rectangular zone. Jacobson (1990) has analyzed the spatial structure of the field saturated hydraulic conductivities from the Las Cruces Trench in detail. Jacobson's analysis indicates that an anisotropic exponential semi-variogram with horizontal and vertical correlation lengths of 2.5 and 0.5 m, respectively, a nugget of 0.4, and a sill of 1.54 adequately fits the sample semi-variogram constructed for the logarithm of hydraulic conductivity. The exponential model with nugget is given by

$$Y(x) = \begin{cases} 0, & x = 0; \\ C_0 + C_1[1 - \exp(x/l)], & x > 0. \end{cases} \quad (4.10)$$

where C_0 is the nugget, C_1 is the sill and l is the correlation length. This semi-variogram was used to krig the saturated hydraulic conductivity. For the other soil hydraulic parameters, the correlation lengths and range determined for the *in situ* K_{sat} were assumed; however, the sill for each

Models

parameter was set equal to its variance. For all hydraulic parameters, kriging was performed in a local neighborhood with a radius of 2.5 m, with 5 nearest neighbors allowed per quadrant.

The computational mesh used for the 9 zone, 121 zone, and 3621 zone models consisted of 81 nodes in the horizontal and 97 nodes in the vertical direction and is shown in Figure 4.1. The mesh was refined towards the center and top of the domain to accommodate the large pressure head gradients expected to occur at early time directly below the strip source. Boundary conditions were defined to be no-flow, except at the bottom of the model and at the 1.2 m horizontal portion located at the top where the strip source is located. To simulate gravity drainage, a negative pressure head gradient of unit magnitude was specified at the bottom of the domain. At the strip source, the prescribed flow boundary condition was set equal to 1.82 cm/day during the first 70 days of simulation and zero thereafter.

All model simulations were performed using the computer code PORFLO-3 (Runchal and Sagar, 1989) on the CRAY Y-MP8/8-64 at Los Alamos National Laboratory (LANL). The PORFLO-3 computer code is a software package designed for solving problems which combine fluid flow, heat transfer and mass transport in variably saturated porous and fractured media. The governing equations for fluid flow, heat transfer and mass transport are spatially discretized using the finite volume or integrated finite difference method. Second order spatial derivatives in the governing equations are integrated assuming a quadratic profile, while first order derivatives in the heat or mass transport equations are integrated using either a quadratic profile or an upwinding scheme. Time discretization is either by an explicit or implicit first order Euler scheme. The resulting nonlinear system of algebraic equations is linearized by the Picard method and solved using either Cholesky decomposition, Gaussian elimination, ADI, or the reduced-system conjugate gradient method. The reduced-system conjugate gradient method was used for the simulations presented here.

4.2 Massachusetts Institute of Technology

Model MIT1

Massachusetts Institute of Technology used a stochastic model to simulate mean water movement for the Plot 2b experiment. The stochastic approach attempts to account for aggregate effects of heterogeneities observed at the field scale on moisture movement and is based on the small perturbation theory developed by Mantoglou and Gelhar (1987a, b, c) and extended by Polmann (1990). By

incorporating the effects of variability in "effective" parameters, one can arrive at an equation describing mean water movement that is similar in form to Richards' equation

$$\frac{\partial E[\theta(H)]}{\partial t} = \frac{\partial}{\partial x_i} \left[K_{ij}^*(H) \frac{\partial (H - x_1)}{\partial x_j} \right] \quad (4.11)$$

where $E[\theta(H)]$ is the effective moisture content, $K_{ij}^*(H)$ is the effective hydraulic conductivity tensor, H is the mean pressure head, and x_j is the cartesian coordinate in the vertical direction.

The effective moisture content is expressed as

$$E[\theta(H)] = \bar{\theta}(H) + \frac{1}{2} \sigma_h^2 \frac{d^2 \bar{\theta}(H)}{dH^2} + E[h\theta'_N] \frac{d\beta_\theta(H)}{dH} \quad (4.12)$$

where $\bar{\theta}(H)$ is the mean moisture content, σ_h^2 is the variance of the capillary tension, $E[h\theta'_N]$ is the cross correlation between fluctuations about the mean tension and fluctuations about the mean moisture content, and β_θ is the standard deviation of fluctuations of moisture content about its mean.

If the anisotropy is aligned with the coordinate system, the vertical and horizontal components of the hydraulic conductivity can be expressed as

$$K_{11}^*(H) = e^{\bar{y} + \frac{\sigma_y^2}{2}} \quad (4.13)$$

$$K_{22}^*(H) = e^{\bar{y} + \frac{\sigma_y^2}{2} + E\left[y' \frac{\partial h}{\partial x_2}\right]} \quad (4.14)$$

where $\bar{y}$ is the mean of the log conductivity, σ_y^2 is the variance of the log conductivity, and $E[y' \frac{\partial h}{\partial x_2}]$ is the cross correlation between fluctuations about the mean conductivity and the spatial gradient of tension. Note that if the variability is zero, the stochastic effective parameters reduce to their deterministic counterparts.

The stochastic effective parameters were estimated from the Las Cruces Database. van Genuchten parameters were estimated from moisture retention data for each of the 450 soil core samples taken on the 9 by 50 grid provided in the database. High tension retention data (≥ 1000 cm)

Figure 4.1. Computational Mesh for the CNWRA Models

Models

determined from the disturbed soil samples were not used because this data was sometimes inconsistent with lower tension data obtained from adjacent core samples. To better match the initial conditions observed in the field, θ_r was constrained to be less than 0.06. Equation (4.4) was used to define the corresponding unsaturated hydraulic conductivity curves.

The set of 450 moisture retention and unsaturated hydraulic conductivity curves were used to estimate the stochastic effective parameters using Marquardt-Levenberg nonlinear regression. The estimation procedures are discussed in Luis (1991). The most noteworthy difference between the stochastic and deterministic effective parameters is the anisotropy ratio exhibited by the hydraulic conductivity. The stochastic effective conductivity exhibits anisotropy that varies with tension, the anisotropy ratio ranging from 1 to approximately 16. For the relative dry conditions simulated here, the ratio ranges from about 3 to 10.

A two-dimensional simulation domain was defined using the uniform soil model defined by the stochastic effective parameters. The domain represents a vertical section parallel to the trench face. Initial moisture conditions provided in the Las Cruces Database were used. An infiltration rate of 1.82 cm/day was applied over the irrigation area for 70 days and the simulation period was 310 days.

Bouloutas (1989) describes the numerical method used here. The numerical model solves the mixed form of Richards' equation using a modified Picard approximation. Temporal discretization is based on a two-step, fully implicit method. Galerkin finite elements with linear basis functions are used to spatially discretize the simulation domain. The spatial step size is 20 cm horizontal by 50 cm vertical. The resulting set of algebraic equations is solved using a preconditioned conjugate gradient method (PCCG). Time step size varies adaptively, increasing when convergence of the PCCG solver is fast and decreasing when it is slow. The simulation was performed on a DECstation 3100.

4.3 New Mexico State University

New Mexico State University used two models for water flow and two models for solute transport. Both models were two-dimensional (x and z directions) and were based on Eqs. (4.1) through (4.7). One of the water flow models assumed a uniform soil while the other assumed a heterogeneous soil. The uniform soil model was based on the van Genuchten parameters and the initial water contents corresponding to the base case defined in the Las Cruces Data Base. The heterogeneous soil model was based on the

van Genuchten parameters that were sampled from the observed spatial distribution of these parameters as defined in the Las Cruces Data Base. Further details are provided below.

The flux updating algorithm of Kirkland et al. (1991) was used to model water flow. This algorithm was developed in-house, is finite difference based, does not require Picard or Newton iteration, is mass conserving, and can handle infiltration into very dry soils. Tritium transport was also modeled in two dimensions (x and z directions) using Eqs. (4.5) through (4.7) using the velocity fields from both water flow models and assuming a uniform retardation factor and dispersivity. The flux corrected transport algorithm in development at NMSU was used to solve the two-dimensional version of Eq. (4.5). This algorithm is finite difference based, can handle heterogeneous, isotropic soils, and can provide useful results for infinite grid Peclet numbers.

Both models were implemented on New Mexico State University's Cray YMP-EL.

4.3.1 Water Flow

Model NMSU1

The simulation domain for the uniform soil model was taken to be 10.1667 m wide by 7 deep. The uniform, isotropic soil model was based on the van Genuchten's curves defined by Eqs. (4.2), (4.3), and (4.4) and the van Genuchten parameters given in the Las Cruces Data Base (Wierenga et al., 1989a):

$$\theta_r = 0.0828, \theta_s = 0.3209, \alpha = 0.05501 \text{ (1/cm)},$$

$$n = 1.5093, K_{sat} = 270.1 \text{ (cm/day)}$$

Cell centered nodes were used with $\Delta x = 0.050833$ m and $\Delta z = 0.05$ m on a $n_x = 200$ by $n_z = 140$ cell mesh where x is measured horizontally to the right and z is measured vertically downward. The initial volumetric water contents as defined for the base case in the Las Cruces Data Base were used. These are given in the files *Base.2m*, *Base.6m*, and *Base.10m* for the 2 m, 6 m, and 10 m planes, respectively. The following procedure was used to define the initial water contents as they appear in these files:

1. When the neutron probe observation points and the finite difference nodes coincided, the observed initial water contents were used. Bilinear interpolation was used to interpolate from the observed initial water contents to the finite difference mesh when the mesh was within the

region covered by the observation nodes. This defined the finite difference nodes $i_x=3,198$; $i_z=6,120$.

2. The water contents for the nodes above the area covered by the observation mesh were set to the finite difference node water contents along the top of that area as defined in item 1. That is, $\theta(i_x, i_z) = \theta(i_x, 6)$; $i_x=3, \dots, 198$; $i_z=1, \dots, 5$.
3. The water contents below the area covered by the observation mesh were set to the finite difference water contents along the bottom of that area as defined in item 1. That is, $\theta(i_x, i_z) = \theta(i_x, 120)$; $i_x=3, \dots, 198$; $i_z=121, \dots, 140$.
4. The water contents to the left and right of the area covered by item 3 were set to the left and right most water contents for the area covered by item 3. That is, $\theta(i_x, i_z) = \theta(3, i_z)$; $i_x=1, 2$; $i_z=1, \dots, 140$ and $\theta(i_x, i_z) = \theta(198, i_z)$; $i_x=199, 200$; $i_z=1, \dots, 140$.
5. Finally, if a water content at a node was below θ_r , it was reset to $1.01\theta_r = 0.0836$ to insure that the initial water content was not lower than θ_r .

Both the uniform soil and the heterogeneous soil models used zero flux boundary conditions on all boundaries except for the center 1.22 m (i.e. the center 24 cells) along the top boundary during irrigation. Water was applied on the 1.22 m wide area at a rate of 1.82 cm/day for the first 70 days of the simulation. The total simulation period was 310 days.

Models NMSU2, NMSU3, NMSU4, NMSU5

A heterogeneous water flow model was also implemented by New Mexico State University using the distributions of hydraulic properties from the Las Cruces Data Base. Four simulations were performed. In all cases, the simulation domain was taken to be 10.1667 m wide by 8 m deep using a finite difference mesh 200 wide by 160 deep. Hydraulic property distributions as measured from four sub-areas of trench face were used for the four simulations. In all cases, the laboratory based rather than the *in situ* based saturated hydraulic conductivities were used. The two-dimensional soil property model for each simulation was generated as follows.

The van Genuchten parameters θ_r , θ_s , α , n and the laboratory based saturated hydraulic conductivities K_{sat} determined for each of the 450 core and disturbed soil sample locations were used. Estimation of these parameters are discussed in Wierenga et al. (1989a). Missing data on

this grid were filled in using inverse-squared weighting interpolation:

$$f_k = \frac{\sum_{m=1}^n w_m f_m}{\sum_{m=1}^n w_m} \quad (4.15)$$

where

$$w_m = \frac{1}{(x_k - x_m)^2 + (z_k - z_m)^2} \quad (4.16)$$

and f_k is the missing hydraulic parameter, f_m are the available values for this hydraulic parameter at the other nodes, and (x_k, z_k) and (x_m, z_m) are the locations of the corresponding nodes. The sum is over n , the total number of locations for which the parameters are available on the 50 by 9 sampling grid.

Given the complete set of parameters on the sampling grid, bilinear interpolation was used to evaluate the parameters for the finite difference grid for the area covered by the 50 by 9 sampling grid.

If the finite difference grid point was outside the sampling grid region, the parameters were set to the values at the closest finite difference mesh point found in the previous step in a fashion similar to that used for the initial water contents as discussed under Model NMSU1.

The basic assumption behind these simulations was that the actual property distribution in some plane away from the trench face was not necessarily the same as along the trench face. Rather than characterizing the property distributions statistically and generating realizations, four realizations were sampled directly from the trench face property distribution. This was done as follows for the NMSU2-NMSU5 models.

NMSU2

The observed two-dimensional property distribution at the trench face from $x=-3.8333$ m to $x=6.3333$ m ($x=0$ corresponds to the actual irrigation area centerline) was used with the procedure discussed above as input to the model with a model domain 10.1667 m wide. The irrigation area was assumed to be centered on the model domain. Thus the simulated irrigation centerline was shifted to the right 1.25 m (+ x direction) relative to the true irrigation for the experiment. The actual left-most sample location for the characterization data is approximately 4 m to the left of the

Models

centerline of the Plot 2b irrigation area. Thus if the property field was taken from the trench face observations without a shift, there would be no values available along the left most side of the simulation domain. The shift of 1.25 m is convenient in that there is no need to extrapolate data to the left of the left-most trench face observations of the hydraulic properties. In addition, there is no significant reason to believe that the property distribution at the trench face with zero shift is a better representation of what is occurring at the neutron probe planes than is a property distribution sampled from the trench face with some small horizontal shift.

NMSU3

The observed two-dimensional property distribution at the trench face from $x=1.1667$ m to $x=11.3333$ m was used as input to the model with a model domain 10.1667 m wide. The irrigation area was assumed to be centered on the model domain. Thus the simulated irrigation centerline was shifted to the right 6.25 m relative to the true irrigation centerline in modeling the experiment.

NMSU4

The observed two-dimensional property distribution at the trench face from $x=6.1667$ m to $x=16.3333$ m was used as input to the model with a model domain 10.1667 m wide. The irrigation area was assumed to be centered on the model domain. Thus the simulated irrigation centerline was shifted to the right 11.25 m relative to the true irrigation centerline in modeling the experiment.

NMSU5

The observed two-dimensional property distribution at the trench face from $x=11.1667$ m to $x=21.3333$ m was used as input to the model with a model domain 10.1667 m wide. The irrigation area was assumed to be centered on the model domain. Thus the simulated irrigation centerline was shifted to the right 16.25 m relative to the true irrigation centerline in modeling the experiment. Note that sampling the realizations in this fashion preserved the actual statistical structure as observed for the trench face.

Since these realizations do not represent the true properties as they occur in the observation planes but are only possible representations, the observed initial water contents were not appropriate for these realizations. As a result, the initial water contents were defined as follows. An average water content for some depth was evaluated using the water contents observed in all three planes ($y=2, 4$, and 6 m) for that depth. At some locations, this average was smaller than the local θ_r . To avoid obtaining a negative relative water content (see Eq. 4.2), the local initial water content was set

equal to the maximum of three quantities; the average water content for that depth, $\theta_r+0.0001$ for that location, or θ as evaluated at 50,000 cm tension using the van Genuchten parameters for that location.

4.3.2 Solute Transport

Tritium transport was modeled using Eq. (4.5) concurrently with water flow so that the water fluxes evaluated using Richards' equation, Eq. (4.1), could be used to define the Darcy fluxes. The retardation factor for tritium R , the molecular dispersion coefficient D_m , and the dispersivity ϵ , were assumed to be constant throughout the entire simulation domain. For all cases

$$R = 1.0$$

$$D_m = 1.0 \text{ (cm}^2\text{/day)}$$

whereas

$$\epsilon = 5 \text{ (cm)}$$

for the uniform soil case (NMSU1) and

$$\epsilon = 3 \text{ (cm)}$$

for the heterogeneous soil cases (NMSU2 through NMSU5). Because the heterogeneous soil model accounts for some of the mechanical dispersion in the velocity field, a lower value for the dispersivity was used.

Transport was modeled concurrently with water flow and the same spatial steps and time steps were used. The initial solute concentrations as defined in the Las Cruces Data Base were used for both the uniform soil and heterogeneous soil models. Bilinear interpolation was used to define initial concentrations at the points between the sampling locations. Zero solute flux boundary conditions were used on all boundaries except for the center 1.22 m of the top boundary during irrigation as discussed above. Solute was applied at a normalized concentration of 0.622 (as specified in Hills et al., 1991) with the irrigation water from day 29 to day 44 of the Plot 2b experiment.

4.4 Pacific Northwest Laboratory

Pacific Northwest Laboratory (PNL) used four models for water flow and two models for solute transport. Two of the water flow models represent uniform, isotropic soil. One of the water flow models represents uniform, anisotropic soil,

and one of the water flow models represents heterogeneous, isotropic soil. All water flow models were two-dimensional and assumed isothermal, single-phase flow conditions.

Flow and transport simulations were conducted using the MSTS code (White and Nichols, 1993; Nichols and White, 1993). MSTS is a three-dimensional, nonisothermal, two-phase flow and transport simulator. The code was developed by PNL in support of the preliminary total system performance assessment of the proposed high-level nuclear-waste repository at Yucca Mountain, Nevada. MSTS uses an integrated finite difference method with a Newton-Raphson iteration scheme. Although MSTS is a multiphase flow and transport code, the equations that were used for these simulations were essentially reduced to those shown previously in Eqs. (4.1) through (4.7), with the exception of the dispersion coefficient formulation shown in Eq. (4.7). The molecular diffusion coefficient in MSTS is multiplied by a saturation-dependent tortuosity factor (Millington and Quirk, 1961), which effectively reduces molecular diffusion as water content decreases.

All simulations were run on a Convex C210 computer. Additional details about the different soil models are described below.

4.4.1 Water Flow

The simulated domains for all of the PNL models represent 11 m wide by 7 m deep vertical cross sections. The modeled domains were discretized using uniform, 0.1 m node spacings in both the horizontal and vertical directions, for a total of 7700 nodes.

Both the uniform and heterogeneous soil models used zero flux boundary conditions on all boundaries except for a 1.2 m wide strip along the center of the top boundary during irrigation and along the bottom boundary. A flux of water equal to 1.82 cm/day was specified for the 1.2 m wide strip during the first 70 days of the simulation period to represent irrigation. A unit hydraulic gradient was specified along the bottom boundary during the entire 310 day simulation period.

The initial water content values measured from all three planes of neutron probe access tubes ($y = 2, 6,$ and 10 m) were used to generate the initial water content distribution for the water flow simulations. Bilinear interpolation was used to interpolate between the measurement locations and nodes in the model grid. Water content values for nodes in the model grid that were outside of the corresponding area of the domain in the measurement grid were assigned values equal to the nearest measured or interpolated value within the measurement or model grid.

Model PNL1

PNL1 represents a uniform, isotropic soil model. The hydraulic properties for this model were represented by combining two sets of van Genuchten (1980b) model parameters. The parameters representing the composite hydraulic property model in the wetter water content range ($\theta > 0.092$) correspond to the parameters used for model NMSU1. These parameters represent the average, best-fit water retention parameters and saturated hydraulic conductivity values determined from laboratory measurements for samples collected from the nine identified soil horizons at the trench site (Hills and Wierenga, 1991). A second set of parameters was used to describe the hydraulic properties of the soil at lower water contents to provide a more accurate representation of the initial conditions of the experiment relative to the parameters used for model NMSU1. The parameters representing the dry-end of the composite hydraulic property model were selected to obtain a smooth transition from the wet to dry regimes, and a water content of approximately 0.0 at a matric potential of 1.0×10^7 cm. The parameters used to represent the composite hydraulic property model are shown below:

For $\theta \leq 0.092$

$$\theta_s = 0.092, \theta_r = 0.0, \alpha = 0.15 \text{ (1/cm)},$$

$$n = 2.5, K_{sat} = 1.0 \times 10^{-8} \text{ (cm/day)}$$

For $\theta > 0.092$

$$\theta_r = 0.0828, \theta_s = 0.3209, \alpha = 0.05501 \text{ (1/cm)},$$

$$n = 1.5093, K_{sat} = 270.1 \text{ (cm/day)}$$

Model PNL2

PNL2 represents a uniform, anisotropic soil model. The hydraulic properties for this model correspond to properties used previously by Kool and Wu (1991) for simulations of the Las Cruces Plot 2a experiment. The water retention parameters for this model were also determined from the average best-fit parameters determined using laboratory data from samples collected from the nine soil horizons. However, the water retention data in the Las Cruces data base were refit, with the values of θ_r constrained during the curve-fitting process to values less than the lowest measured water content in each soil horizon. The saturated hydraulic conductivity in the vertical direction K_z was computed from the average of the laboratory

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measurements, assuming a lognormal distribution as follows:

$$K_x = \exp\left(\mu_{\ln} + \frac{1}{2}\sigma_{\ln}^2\right) \quad (4.17)$$

where $\mu_{\ln}$ and $\sigma_{\ln}$ are the mean and standard deviation, respectively, of the log transformed K_{sat} values of the individual soil cores. The saturated hydraulic conductivity in the horizontal direction K_x was assigned a value twice as large as the vertical direction in an attempt to better reproduce the observed spread of the water plume for the Plot 2a experiment (Kool and Wu, 1991). The parameters used to represent the hydraulic properties for this model are shown below.

$$\theta_s = 0.32, \theta_r = 0.025, \alpha = 0.112 \text{ (1/cm)},$$

$$n = 1.253, K_x = 1310 \text{ (cm/day)}, K_z = 655 \text{ (cm/day)}$$

Model PNL3

PNL3 represents a uniform, isotropic soil model. The van Genuchten model α and n parameters for this model were estimated from a one-dimensional inverse solution using water content data obtained during the first 35 days of infiltration during Las Cruces Plot 1 experiment. The values of θ_s and K_{sat} for this model correspond approximately to the geometric mean values calculated from the full two-dimensional set of laboratory-measured water retention, and field-measured K_{sat} data, respectively. The full two-dimensional data set consists of data from the 9 horizontal sampling transects, as well as data from 3 vertical transects. The value of θ_r was fixed at a value slightly lower than the lowest measured initial water content prior to the Plot 1 experiment. The parameters representing the hydraulic properties for this model are shown below.

$$\theta_s = 0.32, \theta_r = 0.04, \alpha = 0.02176 \text{ (1/cm)},$$

$$n = 1.4956, K_{sat} = 376 \text{ (cm/day)}$$

Model PNL4

PNL4 represents a fully heterogeneous, isotropic soil model. The water retention parameters used for this model correspond to kriged estimates based on the parameters that were refit with constrained values of θ_r , as reported by

Kool and Wu (1991). The saturated hydraulic conductivities for this model were assumed to be isotropic and correspond to a spatially-correlated random field that was conditioned on the field-measured K_{sat} data from the trench. The kriged water retention parameter estimates and K_{sat} conditioning data were generated from, or correspond to, samples collected between the x-coordinates of -3.78 m and 5.22 m in the Plot 2 coordinate system.

All kriged parameter fields were generated assuming an exponential covariance model with horizontal and vertical correlation lengths of 2.5 and 0.5 m, respectively. These correlation lengths and covariance model were estimated from semivariogram analyses by Jacobson (1990). The spatially correlated random hydraulic conductivity field for this case was generated using a fast Fourier transform method.

4.4.2 Solute Transport

Tritium transport was modeled with Eq. (4.5), using the velocity and saturation fields generated from the solution of the flow equation. The retardation factor for tritium, R , was taken to be equal to a constant value of 1.0 throughout the modeled domains for all simulation cases. The coefficient of molecular diffusion, D_m , was taken to be a constant value of $1.0 \text{ cm}^2/\text{day}$ throughout the modeled domains for all simulation cases. As noted previously, the coefficient of molecular diffusion in MSTs is multiplied by a saturation-dependent tortuosity factor (Millington and Quirk, 1961), which effectively reduces molecular diffusion as water content decreases. The dispersivity, ϵ , was also assumed to be constant throughout the modeled domains for all cases, and was assigned a value of 5 cm for models PNL1, PNL2, and PNL3, and value of 0.0 for model PNL4. The mechanical dispersion coefficient was assigned a value of 0.0 for model PNL4 because the variations in the velocity field that are created by using heterogeneous hydraulic properties create a dispersion effect without using a mechanical dispersion coefficient.

The same spatial and time steps that were used for flow simulations were also used for transport simulations. The initial tritium concentrations measured from the solution samplers, which are located 0.5 m from the face of the trench ($y = 0.5 \text{ m}$), were used for initial conditions for all soil models. Bilinear interpolation was used to interpolate from the measurement locations to nodes in the model grid.

Zero solute flux boundary conditions were used on all of the model boundaries except for the 1.2 m wide strip in the center of the upper boundary. A normalized tritium concentration of 0.622 was specified for this part of the top boundary from day 29 through day 44 of the simulated period.

Additional details about the PNL simulations are described by Rockhold (1993).

4.5 The University of Texas

Model BEG1

The Bureau of Economic Geology simulated two-dimensional water flow using the computer code TRACR3D (Travis and Birdsell, 1991). The TRACR3D code solves three-dimensional, isothermal, transient, two phase flow and multicomponent transport in variably saturated porous media. An implicit finite-difference scheme is used to solve the flow and transport equations. TRACR3D includes many features that enhance its ability to converge for highly nonlinear flow problems such as use of the Newton-Raphson iterative scheme, which is more strongly convergent (second order) than the generally used Picard scheme (first order). The code also uses an efficient preconditioned conjugate gradient matrix solver. TRACR3D uses a variable time-stepping scheme based on the number of iterations per time step. The model was implemented on a DEC VAX 3100 work station, a SUN 690 server station and a CRAY YMP 864. The VAX 3100 was used for the simulations presented here.

The model was based on uniform, isotropic soil properties. The van Genuchten parameters are arithmetic means of the values for the individual soil cores. The values of the van Genuchten hydraulic parameters used in this simulation differ from those given in the Las Cruces trench database in that an upper limit was set for the residual water content θ_r in the fitting procedure, based on the lowest measured

water content in each soil layer in the field (Kool and Wu, 1991). Values of the parameters α and n also differ from those in the database because of the differences in the θ_r values. Saturated hydraulic conductivity was based on a geometric mean of individual soil core values.

$$\theta_r = 0.025, \theta_s = 0.3266, \alpha = 0.11183 \text{ (1/cm)},$$

$$n = 1.4062, K_{sat} = 270.1 \text{ (cm/day)}$$

The model domain was 12 m wide by 8 m deep and was represented by a 120 by 70 mesh; therefore, $\Delta x = 0.10$ m and $\Delta z = 0.10$ m from the surface to 6 m depth and $\Delta z = 0.20$ m from 6 to 8 m depth. The initial matric potentials described in the Las Cruces Data Base were used (file TENS2B.DAT). Matric potentials vary smoothly over space whereas water contents can be discontinuous in heterogeneous soils. Procedures similar to those outlined in the description of Model NMSU1 for interpolating and extrapolating the measured water content data were used to obtain the initial matric potentials for the finite difference mesh.

The surface boundary condition that describes the irrigated region was:

$$q(x,t) = \begin{cases} 1.82 \text{ cm/day, } t \leq 70 \text{ days, } -0.6 \text{ m} \leq x \leq 0.6 \text{ m} \\ 0, & \text{otherwise} \end{cases}$$

where q is irrigation rate. The lower boundary matric potential was held fixed at the initial value. The remainder of the boundaries were defined as zero flux.

5 Model Testing Methodology

The comparisons of model predictions and field scale observations for water flow and contaminant transport is critical to the development of confidence in these models. Traditionally, these comparisons have been qualitative, such as through contour plots of the plumes. As the quality and quantity of field data increases, there is increased need to develop more rigorous quantitative model testing methodologies. The choice of the proper quantitative method is not an obvious task since significant uncertainty exists in the characterization of a site's hydraulic properties due to spatial variability. Significant differences between predictions and observations of water content and solute concentrations at point locations are expected and the best that one can hope for is the successful prediction of some sort of mean behavior and an estimate of the statistics of the uncertainty. From a stochastic modeling point of view, mean behavior usually is estimated from ensemble averages of model predictions given many spatial realizations of the property fields. In contrast, a field experiment represents only a single three-dimensional realization of a property field and ensemble averages are not available for comparison to model ensemble averages.

The scales of the solute plumes (≈ 2 m) for the Plot 2b experiment are not significantly greater than the horizontal correlation scales of the spatial heterogeneities. The correlation scales of the saturated hydraulic conductivities were estimated to be 2.5 m by Jacobson (1990). Likewise, water plume widths (≈ 5 to 8 m by day 310) are not sufficiently greater than the correlation scales. The assumption of ergodicity is not justifiable and the uncertainty in the local variability must be accounted for if the model testing procedures are to be fully rigorous. This requires sensitivity or Monte Carlo analysis which is beyond the scope of the present work. Here we limit the comparisons between model predictions and experimental observations to visual comparisons through graphs and through simple, non parametric, statistical tests. As model validation methodologies for non-ergodic systems are developed, the Las Cruces Data Base can be revisited.

5.1 Procedure

The following procedure was used during Phase II of INTRAVAL to generate the model testing data:

1. Using a simple uniform soil, deterministic model, various scenarios for the Plot 2b experiment were

simulated by NMSU to help optimize the water/tracer application rates and durations. The intent was to design the experiment so that the water plume just reached the bottom of the observation domain ($z = 6$ m) and so the leading edge of the tritium that was applied during the Plot 2b experiment just reached the trailing edge of the existing tritium plume from the Plot 2a experiment during the final days of irrigation. Except for NMSU, the modelers were not aware of these design goals.

2. The Plot 2b experiment was performed, and the actual water/tracer application rates, the initial volumetric water contents in the $y = 2, 6,$ and 10 m planes, and the initial normalized solute concentrations in the $y = 0.5$ m plane were provided to the modelers.
3. Using the actual water/tracer application histories, the Plot 2b experiment was simulated by the participating modelers.
4. Several of the modelers provided NMSU with ASCII files of the predicted volumetric water contents and normalized solute concentrations at the measurement locations and times. Since this data was provided to NMSU without the modelers having access to the experimental data, these model predictions were considered blind (see Table 4.1).
5. Preliminary comparisons between experimental data and model predictions were made and presented at an INTRAVAL workshop. The experimental data was then released to those modelers that had supplied the corresponding model predictions to NMSU.
6. Additional model predictions were provided to NMSU after the above presentations were made. We consider these predictions to not be blind (see Table 4.1). To be totally unbiased, we also consider the model predictions provided by NMSU to be non-blind since one of the NMSU personnel had access to the data.

While several chemicals were applied during the execution of the Plot 2b experiment, only tritium was modeled. The data set from tritium proved to be the most complete and deemed to be the most reliable by the experimentalist.

Methodology

As mentioned in item 2, the initial conditions were provided to the modelers. ASCII files for the initial conditions for water content in the $y=2, 6,$ and 10 m planes and tritium in the $y=0.5$ m plane were provided through the Las Cruces Database. Model predictions were returned to NMSU in the same format for the measurement times and locations. Each record of the initial condition and model prediction files included a time (days since start of Plot 2b experiment), the x, y, z coordinates (m) measured relative to the Plot 2b irrigation centerline, and the value of the predicted variable. These files were read using the following single precision FORTRAN segment:

```
I = 1
1  CONTINUE
  READ(9,*,ERR=2) DAY(I), X(I), Y(I), Z(I), VALUE(I)
  I = I + 1
  GO TO 1
2  CONTINUE
```

While we originally requested that the modelers supply additional files that described integrated quantities, such as the location of the center of mass of the plumes as a function of time, we canceled this request and used the point measurement prediction files to generate the integrated quantities. Doing so insured that the techniques used to generate the integrated quantities from the predicted data were identical to those used to generate the integrated quantities from the experimental data.

5.2 Point Comparisons

Scatter plots of observed vs. predicted volumetric water contents and normalized solute concentrations were used to compare point values of these quantities. Scatter plots provide a more realistic assessment of point value predictions than do contour plots because contouring methods inherently (sometimes intentionally) average data and because the resulting contours can be very dependent on the analytical techniques used to generate the contours. Scatter plots have the added advantage of showing the scatter of the observations about the predictions which give a good indication of bias and uncertainty about the mean.

Even with these advantages, care must be taken in interpreting the results from scatter plots. Because the soils at the Las Cruces Trench Site are spatially variable, and because there is uncertainty in the characterization of the spatial distributions of the corresponding hydraulic properties, there must be uncertainty in the model predictions. Significant scatter of the point values of the experimental observations about the model predictions is to be expected with the level of the scatter dependent on the model type. Models that satisfactorily predict mean

behavior are expected to have less scatter of the point experimental data about the model predictions than models that are based on one unconditioned realization of a heterogeneous property field. The mean square difference between two independent random variables with the same statistics is larger than the mean square difference between an estimator of mean behavior (i.e., a model that successfully predicts mean behavior) and the actual behavior (see Eqs. (4) and (5) in Reynolds, 1984).

Contour plots are also presented. While these plots can be misleading in that the results often are very dependent on the contouring algorithm, contour plots are useful in visualizing qualitative behavior.

Plots for times of first arrivals of the water and solute plumes at various depths were also prepared. We defined the time of arrival of the water plume as that time when the volumetric water content increased by 0.03 from the initial conditions in any of the three measurement planes $y = 2, 6,$ and 10 m. Using a smaller value to detect the leading edge of the water plume resulted in false first arrival times due to errors that occasionally occurred during the measurement process. Even though neutron probes are precise instruments, random measurement errors occur due to the stochastic nature of neutron emission, the errors associated with positioning the probe in an access tube, and other human factors. Over $36,000$ water content measurements were used to generate the first arrival time plots presented here. Occasional measurement errors with magnitudes greater than 0.02 or 0.03 can be expected with such large data sets. Data filtering techniques could be used to smooth some of these errors. However, we did not use such techniques here because the choice of the filtering method is somewhat arbitrary when one does not know the probability distributions for the errors. In addition, filtering will smooth the normally steep leading edge of the water plume.

Because a tritium plume existed in the soil profile from a previous experiment, an attempt was made to define some quantitative measure by which the separation depth between the old and new tritium plumes could be estimated. Unfortunately, computer animations of the experimental plumes indicated that the new plume catches the old plume immediately (within the first meter). This is in contrast to the model results used to design the experiment which predicted a clear separation between the two plumes until they moved much deeper into the soil profile. In addition, the maximum concentration of the old plume is small compared to the new plume and the peak of the old plume is very diffuse due to the long time it has resided in the soil. As a result, we were not able to unambiguously define a leading edge of the new plume using the experimental observations. However, the depth where the new plume concentration exceeded the maximum of the old plume

could be easily detected. As a result, we used two detection increments. The movement of the leading edge of the original plume was evaluated using a tritium concentration increment of 0.02. A concentration increment of 0.25 was used to detect the movement of the second plume.

5.3 Integrated Comparisons

Integrated quantities were evaluated to investigate mean behavior. Unlike scatter plots, missing data can affect the validity of integrated measures since the measures presented here are integrated over space. Water content measurement locations were occasionally skipped during the measurement process. Fortunately, the measurement time intervals were chosen such that there was little change in water content between subsequent measurement days. To estimate the skipped values for water content for use in evaluating the integrated quantities (not used for the scatter plots), linear interpolation over time was used. Computer generated animations of the resulting interpolated data showed that linear interpolation lead to reasonable results as the plume movement appeared to be smooth over time. Another source of missing data was due to obstructions that appeared after some time in several of the neutron probe access tubes at depth. The source of these obstructions were unknown, but they tended to form in adjacent tubes at the same depths suggesting that they were caused by some type of local anomaly. Efforts to keep the thin wall aluminum tubes cleared ranged from using desiccant to inhibit corrosion to mechanically removing the blockage using wire brushes and reamers. None of these methods proved to be satisfactory and the efforts to keep the tubes clear were finally abandoned. This resulted in the loss of all measurements below the obstruction depths for all subsequent measurements. In such cases, water content measurements were not included in the Las Cruces Database for these depths and times. Since no measurements were available after, below, or usually to both sides of these locations, it was decided that interpolation would be unreliable and the data must be considered non-recoverable. Fortunately, the number of non-recoverable data points were small compared to the number of successful measurements for water content.

To evaluate integrated behavior of the water plumes, normalized first and second moments as a function of time were calculated as follows:

$$M_x = \frac{1}{M_0} \sum_{i=1}^n x_i \Delta\theta_i \quad (5.1)$$

$$M_z = \frac{1}{M_0} \sum_{i=1}^n z_i \Delta\theta_i \quad (5.2)$$

$$M_{xx} = \frac{1}{M_0} \sum_{i=1}^n x_i^2 \Delta\theta_i - M_x^2 \quad (5.3)$$

$$M_{zz} = \frac{1}{M_0} \sum_{i=1}^n z_i^2 \Delta\theta_i - M_z^2 \quad (5.4)$$

$$M_{xz} = \frac{1}{M_0} \sum_{i=1}^n x_i z_i \Delta\theta_i - M_x M_z \quad (5.5)$$

were

$$M_0 = \sum_{i=1}^n \Delta\theta_i \quad (5.6)$$

and $\Delta\theta_i$ is the change in volumetric water content from day zero of the Plot 2b experiment at measurement node i . The above summations are over all the measurement locations for which measurements are available (either directly or through interpolation). Whenever a measurement was missing and could not be recovered through interpolation, the corresponding model prediction was also not included in its summation for consistency. Thus the moments presented here represent point moments of the available data. These moments diverge somewhat from true integrated moments later in the experiment when some of the neutron probe access tubes became blocked and when the plume moved out of the observable region.

The net change in water content below various horizons were evaluated as a function of time and normalized by total water applied during the experiment.

$$\Delta V(z) = b \sum_{i=1}^{m(z)} \Delta\theta_i \quad (5.7)$$

$$b = \frac{0.25}{0.0182 \times 1.22 \times 70 \times 3} \quad (5.8)$$

The dimensionless constant b is the area represented by a typical measurement node (1.0 m wide by 0.25 m deep) divided by the total water applied during irrigation (0.0182 m/day over a 1.22 m wide area for 70 days) averaged over the 3 planes. The summation is over all nodes for which measurements are available below the depth z of interest.

Methodology

Since ΔV is normalized by the water applied, it should not exceed but should approach unity near the end of the irrigation period.

The ability to take solute samples using the solute samplers in the trench face is highly dependent on the availability of water around the ceramic cups and the absence of air leaks in the sampling system that occur due to degradation of the joints in the samplers and the vacuum system. Low water contents around the porous sampling cups leads to a very small or zero volume of solute sample. In such cases, tritium concentration could not be estimated. Altogether, 3209 successful measurements out of a possible 6600 measurements for tritium concentrations were made over the 310 day time period of the experiment. The spatial distributions of the missing samples were such that it would be unreliable and misleading to use interpolation to estimate the missing data. As a result, the spatial moments for the tritium plumes were not evaluated. However, a quantity that could be evaluated was the net change in relative concentrations below various planes at those points for which concentration measurements were available. In the analysis presented here, only the model predictions for which there were the corresponding experimental observations were used. This insured that an equal number of points were used when comparing the sum of the observed concentration changes to the sum of the predicted concentrations below a specific depth as a function of time. The sum was evaluated as follows

$$\Delta C(z) = \sum_{i=1}^{m(z)} \Delta c_i \quad (5.9)$$

where the summation is over the total number, $m(z)$, of successful observations of tritium concentration below the depth, z , of interest.

5.4 Summary and Implementation

Four FORTRAN programs were written to generate the desired data files, given the point values of the experimental data and model predictions. The experimental data and corresponding model predictions were processed concurrently. Two programs processed the data for water

flow and two processed the data for tritium transport. The programs performed the following tasks:

1. Sort the point values into arrays representing each measurement plane and time.
2. Write the experimental observation/model prediction data pairs for all available measurement locations (all three planes for water and one plane for tritium) to a water file for each of days 0, 70, and 310 and a tritium file for each of the days 70 and 310.
3. Write data files to be used to generate contour plots for water contents in the $y=2$ m plane and for tritium in the $y=0.5$ m plane for days 70 and 310.
4. Evaluate first time of arrivals using all three planes for water and one plane for tritium and write the results to one data file for water and two data files (i.e., the old and new plumes) for tritium.
5. Use linear interpolation over time to fill some of the missing experimental data for water content (see previous discussion).
6. Evaluate the change in the net observed water volume and concentration below the $z = 1, 2, 3, 4$, and 5 m horizons and write the results to a file for water and to a file for tritium.
7. Evaluate the various moments and write the results to a file for water.

Altogether, 8 files were generated for each water flow model and 7 files for each tritium model.

Only data from $-5 \text{ m} \leq x \leq 5 \text{ m}$ were used for the water content comparisons. While measurements were available for water content at $x = \pm 6 \text{ m}$ starting on day 198, initial water contents at $x = \pm 6 \text{ m}$ were not available at the time the initial conditions were distributed to the modelers. As a result, most of the modelers that used the supplied initial condition files simulated a 10 m wide region. To be consistent, all model comparisons were carried out using only the water content data taken from $-5 \text{ m} \leq x \leq 5 \text{ m}$. All of the measurements were used for tritium.

6 Results

Comparisons between model predictions and experimental observations are presented in several formats. These include snap shots in time of point quantities through contour and scatter plots, integrated quantities as functions of time, and first arrival times as functions of depth. The measurement period used for model comparisons was from day 0 to day 310 of the Plot 2b experiment. Water contents and tritium were each taken on 55 days during the 310 day period. Due to the time consuming nature of the water content measurements, solute samples were sometimes taken on different days. To limit the quantity of the results presented here, scatter plots of observed water contents versus predicted water contents only for days 0, 70, and 310 and the corresponding plots for tritium for days 70 and 310 are presented. The scatter plots of the day zero water contents show clear differences in how the models handled the initial conditions. Day 70 represents the last day of irrigation and day 310 is the last day for which the modelers provided data. Contour plots are presented for days 70 and 310. The first arrival times and the integrated quantities, such as plume moments and changes in water volume, utilize data from all 55 measurement days.

6.1 Point Comparisons of Water Content

Scatter plots of the observed versus predicted initial volumetric water contents are shown in Figures 6.1 through 6.4. The figures for this chapter are grouped at the end of the chapter for reader convenience. Except for the CNWRA models and PNL4 (see model descriptions in the previous chapter), the plots show the data from all three measurement planes ($y = 2, 6, 10$ m planes). The CNWRA and PNL4 models are for the $y = 2$ m plane.

As discussed in the Chapter 4, there are considerable differences in how the models handle the initial conditions. These differences are clearly reflected in the scatter plots. Perfect predictions result in all of the data lying on the $\theta_{\text{experiment}} = \theta_{\text{predicted}}$ 45° line. The predicted initial water contents for BEG1 are higher than most of the corresponding observed water contents resulting in most of the plotted data lying below this line. The initial conditions for BEG1 were based on initial tensiometer measurements. Since tensiometers do not operate under dry soil conditions, measurements were not available for the regions outside of the water plume left by the Plot 2a experiment. BEG1 defined the initial tensions for these regions to be equal to those from the nearest available tensiometer measurements. Because the nearest tensiometer measurements were likely

to be in wetter soils, the initial conditions for BEG1 were heavily biased toward higher water contents. The CNWRA and PNL models best represent the initial water contents. As discussed in the previous chapter, considerable effort was made by CNWRA and PNL to modify the van Genuchten water retention models and parameters so that the initial water contents could be modeled accurately. The CNWRA models were discretized such that the measurement nodes corresponded to a subset of the model nodes. The initial conditions at these nodes were set to the observed initial conditions resulting in the exact agreement shown in Figure 6.3. The discrepancies between the observed and modeled initial water contents for the PNL models are due to interpolation. Since the finite difference nodes did not align with the measurement nodes, interpolation was used to map the initial water contents to the finite difference nodes. The resulting nodal values were then interpolated back to the measurement locations for output as model predictions. As a result of this double interpolation, the measured and interpolated model initial water contents were not in exact agreement. The NMSU1 uniform soil model provided better agreement above $\theta = 0.09$ than the PNL models because NMSU1 used a finer grid size for which the double interpolation had a smaller effect. Water contents below the uniform soil model residual water content θ_r could not be handled by NMSU1. When an observed water content was below θ_r , the initial water content was set to $1.01\theta_r (= 0.0836)$ as reflected in Figure 6.1. The NMSU2 through NMSU5 initial water contents were defined based on average water contents at a depth (see the model description in Chapter 4) rather than on observed local values. As a result, there is little agreement between the observed and the corresponding model water contents. MIT did not provide model output for initial water contents.

The corresponding volumetric water contents for Day 70 are presented in Figures 6.5 through 6.8. All models do a poor job of predicting point values of water content. This is expected since there is considerable uncertainty in the hydraulic property distributions at the measurement planes. The uniform soil, layered soil, and effective media models (BEG1, CNWRA1, MIT1, NMSU1, PNL1, PNL2, PNL3) predict mean behavior. Significant differences are expected for these models since there is considerable variation in the local hydraulic properties (see Hills et al. 1991). The heterogeneous soil models that are conditioned on the observed hydraulic property distributions at the corresponding y - z locations at the trench face (CNWRA2, CNWRA3, PNL4) also show significant scatter. This may be because the property distributions at the trench face do

Results

not necessarily reflect the property distributions in the other planes. The heterogeneous soil models that were not conditioned on the properties at the corresponding y-z locations on the trench face (NMSU2-NMSU5) also show considerable scatter.

The volumetric water contents for day 310 are shown in Figures 6.9 through 6.12. Irrigation stopped on day 70 and day 310 corresponds to 240 days of redistribution. Comparing the day 310 plots against the day 70 plots for each model clearly shows that the redistribution, as predicted by the models, leads to a reduction in the range of the predicted water contents. This is especially true for the uniform soil and effective media models (BEG1, MIT1, NMSU1, PNL1-PNL3) for which the maximum water contents predicted on day 310 are considerable less than those predicted on day 70. Uniform soil models predict mean behavior and the resulting spatial variability in water contents is expected to be less than for heterogeneous models. The soil models that possess water retention characteristics that are heterogeneous over space (CNWRA2, CNWRA3, PNL4, NMSU2-NMSU5) show higher maximums and more variability in water content on day 310.

Based on visual inspection of the scatter plots, accurately modeling the initial conditions (i.e., the CNWRA and PNL models) does not appear to lead to significantly better predictions for the heterogeneous models on day 310. However, the statistics of the prediction errors (predicted minus observed water contents) reveal a clearer pattern. Simple statistics for the prediction errors are presented in Table 6.1. Note that while most models have mean and median prediction errors that are small, the CNWRA and PNL models generally possess smaller means and medians. If a model is mass conservative in the sense that the total mass in the observable system is well modeled, then the mean model prediction error over the observable system will be small regardless on how the model distributes this mass across the system. The effect of approximating the initial conditions more accurately is seen in the mean/median statistics for the CNWRA and PNL models. In contrast, BEG1 shows a very strong positive bias in water content of more than 0.06 indicating BEG1 has significantly more water mass in the system than it should.

Table 6.1 also presents the root mean squared (RMS) of the model prediction errors for days 70 and 310. Note that BEG1 shows the largest RMS for days 70 and 310. The uniform soil models, NMSU1, PNL1, and PNL3, show the lowest RMS for day 70. NMSU1 and PNL1 show the lowest RMS for day 310. The model that provided the next largest RMS on day 310 was CNWRA3 which is heterogeneous. There seems to be no clear advantage to conditioning the model properties on the heterogeneities of the spatial property field as the models with the lowest

RMS are uniform soil models. This suggests that the property fields used to condition the heterogeneous soil models were not appropriate for the prediction planes. Uniform soil models that successfully predict mean behavior are expected to have a lower RMS errors than unconditioned heterogeneous soil models (see discussion in Section 5.2).

To obtain a better picture of the nature of the scatter of the prediction errors, box plots for the differences between predicted and observed water contents for days 70 and 310 are shown in Figure 6.13. Each box spans the middle two quartiles of the corresponding sample distributions with the median indicated by the horizontal lines through each box. The whiskers span the entire sample population with the exception of outliers. Data points are considered outliers if their values are either greater than $1.5 * (UQ - LQ) + UQ$ or less than $LQ - 1.5 * (UQ - LQ)$ where UQ and LQ represent the upper and lower quartile points in the population (i.e., the location of the top and bottom of a box). The outliers are denoted by open circles. Note that the populations of differences between model predictions and experimental observations have population medians very close to zero (i.e., < 0.015) for all models except for BEG1. The initial water contents for BEG1 are significantly greater than those observed for the experiment (see Figure 6.1) which leads to a median for the model prediction errors that are significantly different from zero. In fact, zero lies well outside the middle two quartiles for BEG1. Note that the population of differences appears to be symmetric about the median for most of the models. This suggests that these populations may be normally distributed.

To test for normality, the Kolmogorov-Smirnov one-sample test was used. The Kolmogorov-Smirnov test (the IMSL (1987) routine DKSONE) evaluates the probability of a difference from the hypothesized distribution (normal in this case) exceeding the maximum observed difference against the two-sided alternative. The larger the probability, the more likely the sample population is from the hypothesized population. The two-sided probability is taken to be twice the one-sided probability. This is a nearly exact approximation for a two-sided probability of less than 0.2 but becomes a poor approximation for larger probability values. The IMSL routine DKSONE does not allow ties. To eliminate ties, uniformly distributed random noise with a range of $\pm 10^{-10}$ was added to the data. It was found that increasing the range of the random noise by an order of magnitude did not effect the results of the Kolmogorov-Smirnov test. The results for all models for days 70 and 310 are shown in Table 6.2. Note that on day 70, only one model (PNL4) has a prediction error population with probability greater than 0.05 of being normally distributed, whereas for day 310, 8 models have a probability greater than 0.05. It is not clear why this is so.

Table 6.1. Prediction Error Statistics for Water Content Models

Model	Minimum	Maximum	Points	Mean	Median	RMS
Day 70						
BEG1	-0.0602	0.1928	773	0.0641	0.0677	0.0731
CNWARA1	-0.1253	0.1569	263	0.0023	-0.0005	0.0443
CNWARA2	-0.1389	0.1710	263	0.0009	0.0003	0.0418
CNWARA3	-0.1173	0.1910	263	0.0010	0.0002	0.0401
MIT1	-0.1292	0.1288	482	0.0048	0.0062	0.0532
NMSU1	-0.1173	0.1415	773	0.0093	0.0100	0.0358
NMSU2	-0.1067	0.1211	773	0.0079	0.0124	0.0373
NMSU3	-0.1458	0.1203	773	0.0071	0.0124	0.0378
NMSU4	-0.1718	0.1109	773	0.0032	0.0094	0.0398
NMSU5	-0.1416	0.1476	773	0.0027	0.0070	0.0410
PNL1	-0.1208	0.1406	773	-0.0003	0.0000	0.0354
PNL2	-0.1273	0.1523	773	-0.001	0.0005	0.0436
PNL3	-0.1109	0.1007	773	-0.0006	0.0016	0.0307
PNL4	-0.1028	0.1280	263	0.0017	0.0029	0.0391
Day 310						
BEG1	-0.0275	0.1555	756	0.0616	0.0624	0.0689
CNWARA1	-0.0869	0.1173	259	0.0021	0.0000	0.0343
CNWARA2	-0.0767	0.1282	259	0.0027	-0.0004	0.0343
CNWARA3	-0.0884	0.1440	259	0.0017	-0.0010	0.0326
MIT1	-0.1154	0.1006	732	0.0090	0.0104	0.0448
NMSU1	-0.0624	0.1094	756	0.0094	0.0093	0.0290
NMSU2	-0.0762	0.1055	756	0.0080	0.0087	0.0353
NMSU3	-0.1242	0.1150	756	0.0054	0.0074	0.0350
NMSU4	-0.1616	0.1072	756	0.0027	0.0051	0.0358
NMSU5	-0.1226	0.1108	756	0.0002	0.0035	0.0361
PNL1	-0.0697	0.1089	756	0.0006	-0.0004	0.0277
PNL2	-0.1190	0.1193	756	0.0011	0.001	0.0376
PNL3	-0.0932	0.0780	756	-0.0026	0.0008	0.0336
PNL4	-0.1364	0.1565	259	0.0003	-0.0028	0.0552

To statistically evaluate whether the medians of the populations of errors are close to zero (or more strictly, whether the population is distributed symmetrically about zero), the non-parametric Wilcoxon sign rank test (the IMSL (1987) routine DSNRNK) was performed. The non-parametric test was used since it is not clear that the populations of prediction errors for the various models are sampled from the same well defined distributions. The Wilcoxon sign rank test assumes that the distribution for each random variable, X_i , is symmetric, the X_i are independent, with all of the X_i having the same median. Caution must be used in interpreting the results since there is no strong evidence supporting these assumptions for the various models. The results for the Wilcoxon sign test are shown in

Table 6.3. Only the CNWARA and PNL models consistently have a probability greater than 0.05 of possessing a prediction error population median of zero (or more strictly, possessing a symmetric distribution about zero) on both days which is consistent with earlier results. NMSU5 also had a significant probability of a zero prediction error median for day 310. It is interesting to note that NMSU5 was based on the heterogeneous hydraulic field sampled furthest from the irrigation centerline which suggests that this result may be pure coincidence.

Contour plots of water contents for days 70 and 310 are shown in Figures 6.14 through 6.41. Contours for only the region covered by the data are shown. A complete data set

Results

Table 6.2. Two-Sided Kolmogorov-Smirnov Test for Normal Distribution for Water Prediction Errors

Model	Day 70 Probability	Day 310 Probability
BEG1	0.034	0.367
CNWRA1	0.000	0.024
CNWRA2	0.000	0.010
CNWRA3	0.000	0.022
MIT1	0.000	0.043
NMSU1	0.000	0.080
NMSU2	0.018	0.431
NMSU3	0.000	0.116
NMSU4	0.000	0.201
NMSU5	0.022	0.271
PNL1	0.000	0.000
PNL2	0.000	0.000
PNL3	0.000	0.110
PNL4	0.105	0.613

Table 6.3. The Wilcoxon Sign Test for a Zero Population Median for Water Prediction Errors

Model	Day 70 Probability	Day 310 Probability
BEG1	0.000	0.000
CNWRA1	0.327	0.357
CNWRA2	0.469	0.413
CNWRA3	0.412	0.490
MIT1	0.000	0.000
NMSU1	0.000	0.000
NMSU2	0.000	0.000
NMSU3	0.000	0.000
NMSU4	0.000	0.002
NMSU5	0.003	0.146
PNL1	0.483	0.212
PNL2	0.327	0.054
PNL3	0.101	0.065
PNL4	0.140	0.308

for day 70 was not provide by MIT for day 70 and only that region covered by the data was plotted. There were no measurements or predictions provided for the upper 0.25 m of the soil profile. These areas were also left blank by the contour algorithm. While most of the models do a respectable job of capturing the overall behavior of the water plume, a few did not. BEG1 shows more water mass outside the plume than is present in the field and a much stronger downward motion of the plume during

redistribution. MIT1 shows considerably more spreading than field conditions reflect and, as a result, less downward motion of the plume. PNL2 shows very little downward motion of the plume relative to field observations while PNL3 shows a very diffuse plume. The heterogeneous soil models (NMSU2-NMSU5 and CNWRA models on day 310) show some features such as multiple locations of peak water contents and a somewhat dry layer mid-depth, that are somewhat consistent with field observations. PNL4

shows a net lateral motion of the water plume to the left which is not consistent with the experimental results and none of the models predicted the dryness and lateral extent of the dry layer at 3 m. Contour plots of experimental water contents for the other measurement planes (not presented here) show that this dry layer extends throughout the measurement domain. Clearly, the characterization of the trench face properties was not adequate to allow this layer to be accurately predicted. This may be due to limitations in the experimental characterization procedures, the inability of Mualem's model (1976) to predict unsaturated hydraulic conductivity given the van Genuchten parameters and K_{sat} , or simply due to differences between the trench face soil properties and those away from the trench face.

Times of first arrivals of the water plume (defined as the time when local volumetric water content increases by 0.03) as a function of depth are shown in Figure 6.42. Note that even though there is considerable scatter in the scatter plots, the first arrival times show very clear trends. Most of the models over predicted first arrival times to depths of 4.25 m whereas all of the models over predicted first arrival times at depths below 4.25 m. Thus, none of the models are conservative from a regulatory point of view in the sense that they over-predict travel times at greater depths. Computer animations of contour plots for the water plumes (not presented here) show that the experimental plume moves quicker through the mid-depth dry layer than do the predicted plumes which explains why most models over-predict travel time at greater depths. The model that is the most conservative at 6 m is BEG1. BEG1 used an initial water content field that was much wetter than the actual conditions. As a result, the downward movement of the plume was greater due to the associated increase in hydraulic conductivity than for models that simulated the initial water contents more accurately. The second most conservative model for the first arrival time is NMSU5 for day 310. However, this is just one of 4 realizations of the NMSU2-NMSU5 models and this realization is based on the property field taken furthest from the irrigation centerline. It is also interesting to note that the heterogeneous soil models did not always lead to more conservative estimates of first arrivals times than did the uniform soil models.

6.2 Predicted Mean Behavior for Water Flow

The change in water volume below a horizon of depth z , normalized by the total water added through the irrigation system, is shown for 6 depths in Figures 6.43 through 6.48. The MIT model is not included because sufficient data was not provided to evaluate time histories of the change in

water contents and the plume moments. Note that the change in water mass below 0 m for the experiment (Figure 6.43) is very close to unity just after irrigation is complete (day 70) indicating that the neutron probe monitoring system accounts for essentially all of the water added. Also note that the experimental curve for the change in water content is a very smooth function of time. This is due to the averaging effect of taking the sum of many measurements and due to a strong correlation of the data over time. After irrigation, the leading edge of the actual water plume moves below the deepest (6 m) measurement depth. Thus the observed water content decreases during redistribution. While most of the models show general agreement in total water balance (Figure 6.43), as depths become larger (Figures 6.44 - 6.48), more models under predict the increase in water content at latter times. The only model that over predicts the change in water content below 3 m is PNL4 which is probably due to the particular heterogeneous property field built into the model. All models under predict the change in water content below 5 m

The first and second moments of the water plumes are shown in Figures 6.49 through 6.53. Note that PNL4 shows considerable horizontal plume movement to negative values of x (Figure 6.49). Two of the four NMSU heterogeneous model realizations, NMSU2 and NMSU5, show significant horizontal movement in the negative and positive x directions respectively. CNWRA2 shows a somewhat smaller positive x displacement. The remaining models show very little horizontal movement which is in agreement with the experimental data. At early times, the experimental water plume is detected at just a few measurement locations. As a result, the early estimate of the plume moments tends to be noisy and the estimate of the normalization constant (i.e., the zeroth moment) is also very noisy. Thus the ratio of these two quantities is noisy for the experimental plume as indicated in the figures. With the exception of PNL4, all of the models under predict the vertical movement of the center of volume of the plume (Figure 6.50). This is consistent with the results obtained from the previous figures. Figure 6.51 indicates that the second horizontal moment (i.e., the horizontal spreading of the plume) is somewhat under predicted by all of the models except for PNL3 and PNL4. These two models significantly over predict plume spreading during redistribution. PNL3 shows a very diffuse, quickly spreading plume, while PNL4 shows strong spreading to the left. While sufficient data was not provided to generate a time history, the contour plots indicate that MIT1 also over predicts the horizontal plume spreading. Figure 6.52 shows that the PNL2, PNL3, and PNL4 under predict the spreading about the centroid in the vertical direction whereas the remaining models over predict vertical spreading.

Results

6.3 Point Comparisons of Solute Concentration

Scatter plots of tritium concentrations for days 70 and 310 are shown in Figures 6.54 through 6.58 for the PNL and NMSU models. The remaining modelers did not provide tritium concentration predictions. Note that all of the models presented show considerable scatter in concentrations and that no model appears clearly superior. A summary of statistics for the population of prediction errors (predicted concentration minus observed concentration) is provided in Table 6.4. The table indicates that all of the models possess small prediction error means and medians. The uniform soil model PNL1 showed the smallest root mean squared (RMS) for the prediction errors for day 70 while the uniform soil model NMSU1 showed the smallest RMS for the prediction errors for day 310. This suggests that more complex models do not necessarily insure better predictions of tritium transport for this experiment.

Box plots for solute concentration prediction errors are shown in Figure 6.59. Note that different scales were used for the day 310 results. Many of the models clearly are not distributed symmetrically about the median. In addition, the distributions appear to change from day 70 to day 310. To test whether the population of prediction errors are

symmetrically distributed about zero, the Wilcoxon Sign test was performed. The results are shown in Table 6.5. Note that all of the NMSU models and only PNL2 test at greater than 5% significance of possessing a symmetric distribution of prediction errors about zero for both days. This is in contrast to the water flow results where the PNL models consistently proved to be more symmetric indicating a zero median prediction error.

The time of arrivals of the 0.02 increment in tritium concentration (detects the leading edge of the tritium plume already in the soil profile at start of the Plot 2b experiment) and the 0.25 increment in concentration (detects only the new plume) are shown in Figures 6.60 and 6.61. The PNL models over predict the time of arrivals of the initial plume at the larger depths and are thus non-conservative in predicting travel time of tritium to depth. Several of the NMSU models under predict the time of arrivals of the initial tritium plume at these depths and are thus conservative. PNL1 and several of the NMSU models are conservative for the time of arrival of the 0.25 increment of the second tritium plume.

Contour plots of tritium on days 70 and 310 are shown in Figures 6.62 through 6.79. Only the region covered by the data was plotted. The measurement domain was from $z = 0.5$ m to 6.0 m and $x = -2.25$ to 2.25 m. The polygon shape of the experimental results is due to missing data outside

Table 6.4. Prediction Error Statistics for Tritium Transport Models

Day 70						
Model	Minimum	Maximum	Points	Mean	Median	RMS
NMSU1	-0.1283	0.3340	72	0.0012	-0.0004	0.0604
NMSU2	-0.2578	0.3009	72	0.0085	-0.0003	0.0846
NMSU3	-0.4304	0.3373	72	0.0129	-0.0002	0.1125
NMSU4	-0.2815	0.3355	72	0.0127	-0.0003	0.1029
NMSU5	-0.4066	0.3582	72	0.0065	-0.0003	0.1076
PNL1	-0.1605	0.2802	72	0.0091	0.0000	0.0588
PNL2	-0.2290	0.2682	72	0.0052	-0.0002	0.0746
PNL3	-0.1879	0.2736	72	0.0213	0.0009	0.0792
PNL4	-0.3123	0.2779	72	0.0182	0.0007	0.0937
Day 310						
NMSU1	-0.1167	0.1240	38	0.0028	0.0003	0.0425
NMSU2	-0.1439	0.0785	38	-0.0087	-0.0009	0.0426
NMSU3	-0.2121	0.1257	38	-0.0036	0.0004	0.0660
NMSU4	-0.1830	0.2240	38	0.0017	0.0003	0.0682
NMSU5	-0.1736	0.1587	38	-0.0020	0.0009	0.0739
PNL1	-0.1320	0.1267	38	0.0080	0.0017	0.0468
PNL2	-0.0558	0.1600	38	0.0066	-0.0002	0.0461
PNL3	-0.0988	0.1525	38	0.0155	0.0018	0.0550
PNL4	-0.1467	0.1959	38	0.0093	-0.0009	0.0750

Table 6.5. The Wilcox Sign Test for a Zero Population Median for Tritium Prediction Errors

Model	Day 70 Probability	Day 310 Probability
NMSU1	0.068	0.241
NMSU2	0.138	0.150
NMSU3	0.458	0.356
NMSU4	0.335	0.345
NMSU5	0.259	0.269
PNL1	0.181	0.028
PNL2	0.479	0.486
PNL3	0.013	0.046
PNL4	0.029	0.037

the shaded polygon. Note that there is general agreement between many of the models and the experimental results on both days. Several of the uniform and heterogeneous soil models show two side by side concentration peaks qualitatively similar to those observed in the experimental results. As expected, several of the heterogeneous models strongly over predict the downward movement of the solute front and are thus conservative (NMSU3 and NMSU5) whereas the uniform soil models are less conservative. It is interesting to note that the heterogeneous NMSU models for tritium transport did bound the arrival times whereas the NMSU water flow models did not.

6.4 Predicted Mean Behavior for Tritium Transport

The sum of changes in concentrations as a function of time for all measurements is shown in Figure 6.80. Only the prediction points which correspond to available measured concentrations were included in the sums. This insured that the same number and location of the points were used when comparing prediction to observation. In contrast to the

water content results, there is considerable scatter in the experimental data for these calculations. However, there seems to be a strong correlation between prediction and observation. Scatter plots of the sum of the observed concentration below the $z = 0, 1, 2$, and 3 horizons and the corresponding predictions show this correlation (Figures 6.81 through 6.84). Note that the correlation between prediction and observation is surprisingly good considering the scatter shown in the data of Figure 6.80 and considering the scatter in the water content data illustrated in the previous figures. This suggests that solute transport may not be more difficult to predict than water flow for this experiment. As the water content contours indicated, there is a dry layer of soil near 3 m through which the water plume passes quickly. The models did not predict such quick movement through this layer resulting in a consistent under prediction of the rate of vertical water movement. In contrast, little of the new tritium reached this layer during the experiment. It is thus not clear whether the tritium predictions would be as good if the tritium plume had passed through this layer. The better agreement between experiment and model for tritium relative to the water content predictions may be simply due to this effect.

Results

Figure 6.1. Scatter Plots for Water Contents (cm^3/cm^3): Day 0, BEG1, NMSU1

Figure 6.2. Scatter Plots for Water Contents (cm^3/cm^3): Day 0, NMSU2 through NMSU5

Figure 6.3. Scatter Plots for Water Contents (cm^3/cm^3): Day 0, CNWRA1 through CNWRA3

Figure 6.4. Scatter Plots for Water Contents (cm^3/cm^3): Day 0, PNL1 through PNL4

Figure 6.5. Scatter Plots for Water Contents (cm^3/cm^3): Day 70, BEG1, MIT1, NMSU1

Figure 6.6. Scatter Plots for Water Contents (cm^3/cm^3): Day 70, NMSU2 through NMSU5

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Figure 6.7. Scatter Plots for Water Contents (cm^3/cm^3): Day 70, CNWRA1 through CNWRA3

Figure 6.8. Scatter Plots for Water Contents (cm^3/cm^3): Day 70, PNL1 through PNL4

Results

Figure 6.9. Scatter Plots for Water Contents (cm^3/cm^3): Day 310, BEG1, MIT1, NMSU1

Figure 6.10. Scatter Plots for Water Contents (cm^3/cm^3): Day 310, NMSU2 through NMSU5

Results

Figure 6.11. Scatter Plots for Water Contents (cm^3/cm^3): Day 310, CNWRA1 through CNWRA3

Figure 6.12. Scatter Plots for Water Contents (cm^3/cm^3): Day 310, PNL1 through PNL4

Figure 6.13. Box Plots for Water Content Prediction Error Populations

Figure 6.14. Water Content Contours (cm^3/cm^3): Day 70, BEG1

Figure 6.15. Water Content Contours (cm^3/cm^3): Day 70, CNWRA1

Figure 6.16. Water Content Contours (cm^3/cm^3): Day 70, CNWRA2

Figure 6.17. Water Content Contours (cm^3/cm^3): Day 70, CNWRA3

Figure 6.18. Water Content Contours (cm³/cm³): Day 70, MIT1

Figure 6.19. Water Content Contours (cm^3/cm^3): Day 70, NMSU1

Figure 6.20. Water Content Contours (cm^3/cm^3): Day 70, NMSU2

Figure 6.21. Water Content Contours (cm^3/cm^3): Day 70, NMSU3

Figure 6.22. Water Content Contours (cm^3/cm^3): Day 70, NMSU4

Figure 6.23. Water Content Contours (cm^3/cm^3): Day 70, NMSU5

Figure 6.24. Water Content Contours (cm^3/cm^3): Day 70, PNL1

Figure 6.25. Water Content Contours (cm^3/cm^3): Day 70, PNL2

Figure 6.26. Water Content Contours (cm^3/cm^3): Day 70, PNL3

Figure 6.27. Water Content Contours (cm^3/cm^3): Day 70, PNL4

Figure 6.28. Water Content Contours (cm^3/cm^3): Day 310, BEG1

Figure 6.29. Water Content Contours (cm^3/cm^3): Day 310, CNWRA1

Figure 6.30. Water Content Contours (cm^3/cm^3): Day 310, CNWRA2

Figure 6.31. Water Content Contours (cm^3/cm^3): Day 310, CNWRA3

Figure 6.32. Water Content Contours (cm^3/cm^3): Day 310, MIT1

Figure 6.33. Water Content Contours (cm^3/cm^3): Day 310, NMSU1

Figure 6.34. Water Content Contours (cm^3/cm^3): Day 310, NMSU2

Figure 6.35. Water Content Contours (cm^3/cm^3): Day 310, NMSU3

Figure 6.36. Water Content Contours (cm^3/cm^3): Day 310, NMSU4

Figure 6.37. Water Content Contours (cm³/cm³): Day 310, NMSU5

Figure 6.38. Water Content Contours (cm^3/cm^3): Day 310, PNL1

Figure 6.39. Water Content Contours (cm^3/cm^3): Day 310, PNL2

Figure 6.40. Water Content Contours (cm^3/cm^3): Day 310, PNL3

Figure 6.41. Water Content Contours (cm^3/cm^3): Day 310, PNL4

Figure 6.42. Time of Arrivals of Water Plume

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Figure 6.43. Normalized Change in Water Volume below $z = 0$ m

Figure 6.44. Normalized Change in Water Volume below $z = 1$ m

Figure 6.45. Normalized Change in Water Volume below $z = 2$ m

Figure 6.46. Normalized Change in Water Volume below $z = 3$ m

Figure 6.47. Normalized Change in Water Volume below $z = 4$ m

Figure 6.48. Normalized Change in Water Volume below $z = 5$ m

Results

Figure 6.49. x-Moment of Water Plume

Figure 6.50. z-Moment of Water Plume

Results

Figure 6.51. xx-Moment of Water Plume

Figure 6.52. zz -Moment of Water Plume

Figure 6.53. xz-Moment of Water Plume

Figure 6.54. Scatter Plots for Normalized Tritium Concentrations: NMSU1, NMSU2

Figure 6.55. Scatter Plots for Normalized Tritium Concentrations: NMSU3, NMSU4

Figure 6.56. Scatter Plots for Normalized Tritium Concentrations: NMSU5, PNL1

Figure 6.57. Scatter Plots for Normalized Tritium Concentrations: PNL2, PNL3

Figure 6.58. Scatter Plots for Normalized Tritium Concentrations: PNL4

Figure 6.59. Box Plots for Tritium Concentration Prediction Error Populations

Figure 6.60. Time of Arrivals of First Tritium Plume (0.02 Increment)

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Figure 6.61. Time of Arrivals of Second Tritium Plume (0.25 Increment)

Figure 6.62. Normalized Tritium Concentration Contours: Day 70, NMSU1

Figure 6.63. Normalized Tritium Concentration Contours: Day 70, NMSU2

Figure 6.64. Normalized Tritium Concentration Contours: Day 70, NMSU3

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Figure 6.65. Normalized Tritium Concentration Contours: Day 70, NMSU4

Figure 6.66. Normalized Tritium Concentration Contours: Day 70, NMSU5

Figure 6.67. Normalized Tritium Concentration Contours: Day 70, PNL1

Figure 6.68. Normalized Tritium Concentration Contours: Day 70, PNL2

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Figure 6.69. Normalized Tritium Concentration Contours: Day 70, PNL3

Figure 6.70. Normalized Tritium Concentration Contours: Day 70, PNL4

Figure 6.71. Normalized Tritium Concentration Contours: Day 310, NMSU1

Figure 6.72. Normalized Tritium Concentration Contours: Day 310, NMSU2

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Figure 6.73. Normalized Tritium Concentration Contours: Day 310, NMSU3

Figure 6.74. Normalized Tritium Concentration Contours: Day 310, NMSU4

Figure 6.75. Normalized Tritium Concentration Contours: Day 310, NMSU5

Figure 6.76. Normalized Tritium Concentration Contours: Day 310, PNL1

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Figure 6.77. Normalized Tritium Concentration Contours: Day 310, PNL2

Figure 6.78. Normalized Tritium Concentration Contours: Day 310, PNL3

Figure 6.79. Normalized Tritium Concentration Contours: Day 310, PNL4

Figure 6.80. Change in the Sum of Normalized Tritium Concentrations below $z = 0$ m

Figure 6.81. Scatter Plots of the Sum of Normalized Tritium Concentrations below $z = 0$ m

Figure 6.82. Scatter Plots of the Sum of Normalized Tritium Concentrations below $z = 1$ m

Figure 6.83. Scatter Plots of the Sum of Normalized Tritium Concentrations below $z = 2$ m

Figure 6.84. Scatter Plots of the Sum of Normalized Tritium Concentrations below $z = 3$ m

7 Conclusions

The testing of models using data from dry, spatially variable soils is not a trivial task. Not only is it difficult to characterize the site, but it is difficult to obtain sufficient high quality solute samples to obtain good estimates of the movement of solute plumes as a function of time. In contrast, water flow in unsaturated soils is easier to monitor. Neutron probes allow water to be monitored at many locations and the measurements are very consistent day to day over periods of years. For the Plot 2b experiment, the total increase in water observed by the neutron probe just after irrigation was very close to the actual water applied (less than 1% error) suggesting that given the spatial variability of the site, the number and location of the neutron probe measurement was sufficient to resolve the water plume.

There are considerable differences in model predictions even though all the modelers had access to the same very large characterization data set for the Las Cruces Trench experiments. Some of the models presented were fairly simple and assumed uniform soil hydraulic property fields while others conditioned the soil models on the observed two-dimensional spatial heterogeneities observed in the trench face. Even though many models were considered, none of the models stood out as clearly superior. All of the models under predicted first arrival times of the water plume at depths greater than 4.5 m and the models that tended to do well by one measure of mean behavior would often perform poorly by another. Since the probability distributions of the prediction errors do not appear to be well defined and were not clearly distributed as normal or log-normal for all of the models considered, parametric statistical tests were not performed. Less powerful non-parametric tests were used. As a result of these quantitative and graphical comparisons, several observations can be made:

1. The CNWRA and PNL models consistently provided better predictions of mean or median water contents (i.e., near zero mean or median predictions errors) which suggested a good accounting for the total mass in the system. This was likely due to the extra care CNWRA and PNL exercised in modeling the actual spatial distribution of the initial water contents. However, the improvement in mass balance that resulted did not necessarily lead to a reduction in the spread of the population prediction errors (i.e. RMS error) about zero relative to the other models. NMSU1, for example, showed a lower RMS than the CNWRA models. Thus accurately modeling the initial conditions does not, in itself, always lead to improved predictions for water flow.
2. Time of first arrival times of the water plume were greater for the experiment than for any of the models once the plume reached 4.5 m. This indicates that none of the models provided conservative estimates for these travel times from a regulatory point of view since they all over-predicted these times. While this is expected for the uniform soil models since they predict mean behavior, this was not expected to be always true for the heterogeneous soil models. Contour plots of experimental water contents show that a dry layer extends throughout the measurement domain. This layer was not well-predicted by any of the models. It is not clear whether this is due to limitations in the experimental characterization procedures, the inability of Mualem's model (1976) to predict unsaturated hydraulic conductivity for this soil layer given the van Genuchten retention model (1980a), or simply due to differences between the soil properties at and away from the trench face.
3. The observed change in the volume of water below all depths greater than 3 m was significantly greater than that predicted by all of the models except for PNL3. While PNL3 was conservative from a regulatory point of view in the sense that it over predicted the change in water content at depth, its behavior during redistribution was considerably different from that observed in the experiment. The predicted water plume was much more diffuse than the observed plume and more horizontal spreading was predicted. The hydraulic parameters used by PNL3 were obtained with an inverse procedure (Rockhold, 1993) using the experimental observations obtained during infiltration for the Plot 1 experiment. In contrast, the soil characterization used by the other models was based on outflow data obtained from core and disturbed soil samples. This may explain why the other models (except MIT1) performed better during redistribution.
4. The two models, PNL2 and MIT1, conceptualized the soil as anisotropic. MIT1 over-predicted the water plume spreading and under-predicted vertical plume movement as did PNL2. PNL2 assumed that the horizontal hydraulic conductivity

Conclusions

was twice the vertical whereas MIT1 used a tension dependent anisotropy derived from stochastic theory. For the first 310 days of the experiment, neither model seemed appropriate. The more conventional isotropic models performed as well or better. However, significant heterogeneity induced anisotropy may be present later in redistribution when the plume becomes larger and when the gravitational forces become less important relative to the matric potential forces.

5. The initial water contents used in the BEG1 model were significantly larger than those observed in the field. While this had the effect of accelerating the downward motion of the water plume which gave good first arrival time estimates, BEG1 performed poorly by many of the other measures.
6. Results from Phase I of INTRAVAL for the Plot 2a experiment suggested that water movement was easier to model than tritium transport (Voss and Nicholson, 1993). However, most of the model comparisons made during the Plot 2a experiment were side by side comparisons of smoothed contour plots. The more extensive comparisons made here do not support this hypothesis. Tritium transport predictions for the Plot 2b experiment were more acceptable than the corresponding water flow predictions in the sense that the observed tritium behavior (first arrival times, change in tritium concentrations below a horizon) was bounded by the various model predictions whereas the observed water flow was not. It is not clear if this is because tritium transport occurs in the wetter portion of the water plume or simply because the tritium plume did not pass through the anomalous dry layer at 3 m.

7. The present results indicate that models that appear superior or conservative (from a regulatory point of view) for water flow do not necessarily lead to superior or conservative predictions for tritium transport. For example, the PNL models generally gave better predictions of mean or median water contents while the NMSU models generally gave better predictions of mean or median solute concentrations. Only PNL4 provided conservative estimates of first arrival time down to 4 m for the water plume. In contrast, only the heterogeneous NMSU3 and NMSU4 models provided conservative estimates of first arrival times for the tritium plume introduced during the Plot 2a experiment whereas the heterogeneous models NMSU3 and NMSU5 and the uniform soil model PNL1 provided conservative estimates of arrival time of the plume introduced during the Plot 2b experiment. These results support the idea that using multiple realizations of heterogeneous soil models (i.e., NMSU2-NMSU5) is an appropriate way to bound contaminant plume behavior.

Overall, the results of the present work show that for this particular experiment, traditional uniform soil or heterogeneous soil models conditioned on detailed site characterization data can predict the overall features of water flow and tritium transport. Even though there are considerable differences in how the models conceptualized the soil profile, no model was clearly superior overall. Superior models by one measure were not always superior by another. This suggests that the effect of characterization uncertainty, even when the site is characterized as thoroughly as the Las Cruces Trench Site, may have a greater impact on model predictions than differences in how the models conceptualize the soil.

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