*Software Requirements, Design,
and Verification and Validation
for the FEHM Application —
A Finite-Element Heat- and
Mass-Transfer Code*

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Software Requirements, Design, and Verification and Validation for the FEHM Application— A Finite-Element Heat- and Mass-Transfer Code

by

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ABSTRACT

The requirements, design, and verification and validation of the software used in the FEHM application, a finite-element heat- and mass-transfer computer code that can simulate nonisothermal multiphase multicomponent flow in porous media, are described. The use of this code is applicable to natural-state studies of geothermal systems and groundwater flow. A primary use of the FEHM application will be to assist in the understanding of flow fields and mass transport in the saturated and unsaturated zones below the proposed Yucca Mountain nuclear waste repository in Nevada. Chapter I describes the software requirements specification for the FEHM application, including the functional and external interface requirements. This specification motivates the software design, discussed in Chapter II, which covers functional requirements, input/output files and associated variables, and error and warning conditions with their associated messages. Chapter III, "Verification and Validation Plan," outlines the manner in which rigorous and complete testing of the model is to be carried out. Whenever possible, the testing will be against known analytical solutions of the same problem, or for more complex test cases for which no analytical solution exists, the code will be benchmarked against the results of other numerical models. The test cases to be performed are detailed and acceptance criteria that must be satisfied are listed. Chapter IV discusses those test cases and describes the results. The cases covered include tests of separate model components, such as the thermodynamic functions or heat conduction, and tests of a more complex nature, such as dry-out of a partially saturated medium, fracture transport with matrix diffusion, multisolute transport with chemical reaction, and three-dimensional radionuclide transport with decay chain. The test of the DOE Code Comparison Project, Problem Five, Case A, which verifies that FEHM has correctly implemented heat and mass transfer and phase partitioning, is also covered.

1.0 PURPOSE

The FEHM application consists of a finite-element-based numerical simulator of nonisothermal, multiphase, multicomponent flow and solute transport in porous media. The FEHM code will be used for parameter sensitivity studies in the design and specification of field tracer and flow experiments and the interpretation of those field experiments. In addition, it will be used for field-scale simulations of radionuclide migration in the saturated and unsaturated zones below the proposed nuclear waste repository at Yucca Mountain, Nevada.

This document includes the following four main chapters:

- **I. Software Requirements Specification.** This chapter documents the functional requirements for the FEHM application that are used in designing the application. Subsequent baseline studies (described in Chapter IV, "Verification and Validation Report") are used to verify that the application fully implements these requirements.
- **II. Software Design.** The design of the FEHM software is described, including functional requirements, input/output files and associated variables, and error and warning conditions with associated messages.
- **III. Verification and Validation Plan.** The Verification and Validation effort tests the options and features of the FEHM application to verify that the requirements specified in Chapter I, "Software Requirements Specification," are satisfied. The approach is to consist of rigorous and complete testing of the model, whenever possible, against known analytical solutions of the same problem or, for more complex test cases for which no analytical solution exists, of benchmarking the code against the results of other numerical models. This chapter details the test cases to be performed, many of which were developed for prior versions of FEHM (Zyvoloski et al. 1992; Zyvoloski and Dash 1991a, 1991b), and lists the acceptance criteria that must be satisfied.
- **IV. Verification and Validation Report.** This chapter discusses the test cases described in "Verification and Validation Plan" and details the results of those tests.

2.0 DEFINITIONS AND ACRONYMS

2.1 Definitions

FEHM: Finite-element heat- and mass-transfer code (Zyvoloski et al. 1988).

FEHMN: an earlier version of FEHM designed specifically for the Yucca Mountain Site Characterization Project. Both versions are now equivalent, and the use of FEHMN has been dropped.

2.2 Acronyms

DOE - U. S. Department of Energy

DKM - double-porosity/double-permeability method

ECM - equivalent continuum method

LANL - Los Alamos National Laboratory

LU - lower-upper

USGS - United States Geological Survey

V&V - verification and validation

YMP - Yucca Mountain Site Characterization Project

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Chapter I:

Software Requirements Specification

1.0 INTRODUCTION

1.1 Purpose

This chapter, "Software Requirements Specification," documents the functional and performance requirements for the FEHM application. It shall be used in designing and implementing the requirements for the application and shall be employed in subsequent baselines to verify that the application has fully implemented these requirements.

1.2 Scope

The FEHM application is based on a finite-element heat- and mass-transfer code that simulates nonisothermal, multiphase, multicomponent flow, and solute transport in porous media. It is applicable to natural-state studies of geothermal systems and groundwater flow. The FEHM code will be used for parameter sensitivity studies in the design and specification of field tracer and flow experiments and the interpretation of those field experiments. In addition, it will be used for field-scale simulations of radionuclide migration in the saturated and unsaturated zones below Yucca Mountain.

2.0 GENERAL DESCRIPTION

2.1 Software Perspective

FEHMN is a version of FEHM (Zyvoloski et al. 1988) that was developed for the C-wells project in the mid 1980s when LANL was analyzing the early well test data of the USGS. Most of the development of FEHM was done while one of the authors (Zyvoloski) was a participant of the Los Alamos Hot Dry Rock Project.

FEHM and FEHMN are aliases that represent the same computer code, and henceforth, the code will be referenced by the simpler acronym, FEHM.

2.2 Software Functions

The major software functions of FEHM are

- calculate finite-element coefficients for a mesh that represents the porous and permeable medium;
- formulate the transient equations for heat conduction, heat and mass transfer for multiphase flow within porous and permeable media, noncondensable gas flow within porous and permeable media, and transport of multiple solutes within porous and permeable media;
- apply constitutive relationships for pressure- and temperature-dependent fluid properties, air/gas properties, relative permeabilities and capillary pressures, reactive and sorbing solutes, dual porosity, double porosity/double permeability, and stress-dependent properties;
- compute the finite-element solution to the transient equations;
- represent the simulation input and output results in a suite of data files;

- perform a restart calculation in which the progress of the flow field is simulated starting at the time and conditions at which a previous run terminated.

2.3 User Characteristics

The user should have experience in reservoir engineering, hydrology, or porous media flow. The user should also have experience with numerical simulations.

2.4 General Constraints

Problem size and limits are dictated by the capabilities of the computer on which the simulation is run. The code shall be able to handle extreme property changes (e.g., large changes in permeability between adjacent strata or highly nonlinear characteristic curves) and systems containing both saturated and unsaturated regions. Provided that the user supplies physically meaningful parameter values, does not violate model assumptions, and runs problems of the type presented in the verification report, results should be reliable.

2.5 Assumptions and Dependencies

FEHM will be written in Fortran 77. It will be developed to run on CRAY and SUN computers. (FEHM has been successfully run on CRAY, SUN, VAX, HP (Unix-based) and IBM RISC computers.) FEHM requires 64-bit precision.

3.0 FUNCTIONAL REQUIREMENTS

Each section below in this chapter deals with a major function enumerated in Section 2.2 above. After a user formulates a problem to be modeled, a mesh representing the physical media would be generated. Data describing the finite-element mesh would be input (Section 3.5) and the element coefficients computed (Section 3.1). Data describing the physical properties of the media and the fluid/gas system to be modeled would be input (Section 3.5). The appropriate finite-element equations would be formulated (Section 3.2) and constitutive relationships applied (Section 3.3). The solution would then be computed (Section 3.4) and results and restart data output (Sections 3.5 and 3.6).

3.1 Finite-Element Coefficient Generation

3.1.1 Introduction

The application shall include routines for the generation of finite-element coefficients. These coefficients represent the purely geometric part of the numerical analog of the partial differential equations that describe the coupled flow processes in porous media. These coefficients include the volume associated with each grid point as well as an area/distance term for all internode pairs. In standard finite-element terminology, this process results in the geometric components of the stiffness matrix.

3.1.2 Inputs

The following data are required to generate the finite-element coefficients:

- the problem dimension (2 or 3 dimensions) and geometry;
- the number of nodes and elements used to define the solution space;

- the node number and x-, y-, and z-coordinates of each node in the finite-element mesh;
- the number of nodes per element (3-noded triangles or 4-noded quadrilaterals for 2-D problems and 4-noded tetrahedrals, 6-noded triangular prisms, or 8-noded quadrilateral polyhedrons for 3-D problems); and
- the element number and nodal connectivity (which nodes define the element) for each element using a right-handed coordinate system.

3.1.3 Processing

The calculation of the finite-element coefficients is accomplished by using the coordinate and element data (type and node list) to develop the connectivity of the node points and volumes and areas associated with the node points. These calculations are first done on an element level and then combined on a node level.

3.1.4 Outputs

Data structures containing the finite-element coefficients for the input mesh shall be output. The volume of each grid point is contained in an array indexed by node number. The area/distance terms are in arrays indexed by the connectivity structure of the grid. This structure is the same as that containing the neighboring nodes of the grid points.

3.2 Formulate Transient Equations

The transient equations shall be formulated, and the system of equations derived from the finite-element representation of the overall mathematical model shall be solved.

3.2.1 Heat-conduction equations

3.2.1.1 Introduction

FEHM shall be capable of simulating the conduction of heat without the flow of any fluids. The basic governing equation is

$$-\bar{\nabla} \cdot (K \bar{\nabla} T) + q + \frac{\partial A_e}{\partial t} = 0 , \quad (1)$$

where K is an effective thermal conductivity, T is the temperature, A_e is the energy per unit volume, and q is the specified energy source term.

3.2.1.2 Inputs

All property and parameter values implied by Eqn. (1) are required as inputs: density, enthalpy, specific heat, thermal conductivity, initial temperatures, boundary values, coordinates of the computational mesh points, and element definitions.

3.2.1.3 Processing

The time derivatives in Eqn. (1) shall be discretized using the standard first-order method (Hinton and Owen 1979) given by

$$f(t^{n+1}) = f(t^n) + \Delta t [af'(t^{n+1}) + (1-a)f'(t^n)] \quad , \quad (2)$$

where $f(t^{n+1})$ is the desired function at time t^{n+1} , $f(t^n)$ is the known value of f at time t^n , Δt is the time step, f' is the derivative of f with respect to time, and a is a weighting factor. The space derivatives in the governing equation shall be discretized using the finite-element formulation (Hinton and Owen 1979). Using numerical integration, the shape-function coefficients for the discretized equations shall be generated at each node.

3.2.1.4 Outputs

The outputs shall be the equation coefficients for the finite-element formulation of the governing equation (Eqn. (1)) at each node.

3.2.2 Heat- and mass-transfer equations

3.2.2.1 Introduction

FEHM shall also be capable of simulating the transport of heat and mass within porous and permeable media. The conservation equations for heat and mass transfer are

$$\begin{aligned} & -\bar{\nabla} \cdot (D_{mv} \bar{\nabla} P_v) - \bar{\nabla} \cdot (D_{ml} \bar{\nabla} P_l) + q_m + \\ & \frac{\partial}{\partial z} g(D_{mv} \rho_v + D_{ml} \rho_l) + \frac{\partial A_m}{\partial t} = 0 \end{aligned} \quad (3)$$

and

$$\begin{aligned} & -\bar{\nabla} \cdot (D_{ev} \bar{\nabla} P_v) - \bar{\nabla} \cdot (D_{el} \bar{\nabla} P_l) - \bar{\nabla} \cdot (K \bar{\nabla} T) + \\ & q_e + \frac{\partial}{\partial z} g(D_{ev} \rho_v + D_{el} \rho_l) + \frac{\partial A_e}{\partial t} = 0 \quad , \end{aligned} \quad (4)$$

where D is the transmissibility, K is an effective thermal conductivity, P is the pressure, T is the temperature, A_m is the mass per unit volume, A_e is the energy per unit volume, q represents the source and sink terms (such as bores, reinjection wells, or groundwater recharge), ρ is the density, z is oriented in the direction of gravity, and g represents the acceleration due to gravity. Here, also, the subscripts v and l indicate quantities

for the vapor phase and the liquid phase, respectively, and the subscripts m and e refer to mass and energy, respectively.

3.2.2.2 Inputs

The inputs required are all property and parameter values implied by Eqns. (3) and (4): permeabilities, porosities, viscosities, densities, internal energies, specific heats, enthalpies, thermal conductivities, initial pressures, initial temperatures, initial saturations, boundary values, coordinates of the computational mesh points, and element definitions.

3.2.2.3 Processing

The time derivatives in Eqns. (3) and (4) shall be discretized using Eqn. (2). The space derivatives in the governing equations shall be discretized using the finite-element formulation (Hinton and Owen 1979). Using numerical integration, the shape-function coefficients for the discretized equations shall be generated at each node.

3.2.2.4 Outputs

The outputs shall be the equation coefficients for the finite-element formulation of the governing equations (Eqns. (3) and (4)) at each node.

3.2.3 Noncondensable gas flow equations

3.2.3.1 Introduction

In addition to the flow of heat and mass, FEHM shall also be capable of simulating noncondensable gas flow (usually air). The noncondensable gas conservation equation is given by

$$-\bar{\nabla} \cdot (C_v D_{mv} \bar{\nabla} P_v) - \bar{\nabla} \cdot (C_l D_{ml} \bar{\nabla} P_l) + q_c + \frac{\partial}{\partial t} g(C_v D_{mv} \rho_v + C_l D_{ml} \rho_l) + \frac{\partial A_c}{\partial t} = 0. \quad (5)$$

Here, C is the concentration of the noncondensable gas, expressed as a fraction of total mass, q_c is the source (or sink) strength, and A_c is the accumulation term.

3.2.3.2 Inputs

The inputs required are all property and parameter values implied by Eqn. (5): gas concentrations, permeabilities, porosities, viscosities, densities, initial pressures and saturations, boundary values, coordinates of the computational mesh points, and element definitions.

3.2.3.3 Processing

The time derivatives in Eqn. (5) shall be discretized using Eqn. (2). The space derivatives in the governing equation shall be discretized using the finite-element formulation (Hinton and Owen 1979). Using numerical integration, the shape-function coefficients for the discretized equations shall be generated at each node.

3.2.3.4 Outputs

The outputs will be the equation coefficients for the finite-element formulation of the governing equation (Eqn. (5)) at each node.

3.2.4 Solute-transport equations

3.2.4.1 Introduction

FEHM shall also be capable of simulating solute transport and shall allow for simultaneous solution of multiple, interacting solutes. The passive solute equations are not directly coupled to the pressure field but use the pressure field obtained by the heat- and mass-transfer solution. The transport equation for a given component is given by

$$-\bar{\nabla} \cdot (C_v D_{mv} \bar{\nabla} P_v) - \bar{\nabla} \cdot (C_l D_{ml} \bar{\nabla} P_l) - \bar{\nabla} \cdot (D_c \bar{\nabla} C_l) + q_c + \frac{\partial}{\partial z} g(C_v D_{mv} \rho_v + C_l D_{ml} \rho_l) + \rho_r \frac{\partial C_R}{\partial t} + \frac{\partial A_c}{\partial t} = 0 \quad (6)$$

Here, C is the concentration of the solute. The additional terms from those in Eqn. (5) are $\bar{\nabla} \cdot (D_c \bar{\nabla} C_l)$, the dispersion term,

and $\rho_r \frac{\partial C_R}{\partial t}$, the adsorption term. C_R represents the adsorption

of species onto the porous media. In addition, the term q_c includes the source or sink due to chemical reaction. The formulation for multiple interacting species used to compute this term is outlined in Section 3.3.6.

3.2.4.2 Inputs

The required inputs are all property and parameter values implied by Eqn. (6): solute concentrations, permeabilities, porosities, viscosities, densities, initial pressures and saturations, boundary values, coordinates of the computational mesh points, and element definitions.

3.2.4.3 Processing

The time derivatives in Eqn. (6) shall be discretized using Eqn. (2). The space derivatives in the governing equation shall

be discretized using the finite-element formulation (Hinton and Owen 1979). Using numerical integration, the shape-function coefficients for the discretized equations shall be generated at each node.

3.2.4.4 Outputs

The outputs shall be the equation coefficients for the finite-element formulation of the governing equation (Eqn. (6)) at each node.

3.2.5 Particle-tracking module

3.2.5.1 Introduction

FEHM shall be capable of simulating solute transport in either the liquid or gas phases using a cell-based particle-tracking algorithm. The algorithm shall be developed to handle either steady-state or transient flow fields for either an equivalent continuum or dual-permeability flow field. The algorithm shall include the following transport submodels:

- dispersion, to be simulated by applying a correction to the time of a particle in a cell based on a transfer function described by a solution to the one-dimensional advective-dispersion equation;
- sorption, using an equilibrium, linear sorption or " K_d " model;
- matrix diffusion with sorption on either the fracture faces or the matrix rock, implemented using the transfer-function approach similar to the method described above for dispersion, with a one-dimensional matrix-diffusion submodel; and
- radioactive decay.

3.2.5.2 Inputs

The required inputs shall be:

- internode mass fluxes and the fluid storage at each node;
- the injection history for particles; and
- transport parameters for the solute, including sorption coefficients, radioactive decay constants, dispersion coefficients, and diffusion coefficients.

3.2.5.3 Processing

Using the inputs listed above, the code shall track the progress of particles from node to node subject to the transport processes of diffusion, dispersion, and sorption. At specified times, the code shall supply the particle concentrations at each node, and at the final time of the simulation, the code shall output the information on each particle such that a restart of the calculation can be performed.

3.2.5.4 Outputs

The outputs shall be the time-varying locations and concentrations of particles.

3.2.6 Sources and sinks

3.2.6.1 Introduction

The following types of sources and sinks shall be implemented:

- specified flow rate;
- specified pressure condition;
- specified heat flux;
- specified temperature;
- specified flux and saturation;
- specified water flux and air pressure;
- specified air flux (no water flow);
- specified water flux (no air flow);
- specified relative humidity of the gas phase; and
- specified air pressure and saturation.

3.2.6.2 Inputs

For each source/sink (depending on source/sink type), the required inputs are

- source/sink location;
- source/sink strength;
- flowing pressure;
- enthalpy or temperature of the fluid injected;
- species concentration in the fluid injected;
- impedance;
- thermal resistance;
- saturation;
- relative humidity; and
- air pressure.

3.2.6.3 Processing

Processing shall consist of determine the pressure, mass flow rate, heat flow, species concentration, saturation, or air flux at each source/sink.

3.2.6.4 Outputs

The outputs shall be pressure, mass flow rate, heat flow, species concentration, saturation, or air flow at each source/sink.

3.3 Apply Constitutive Relationships

The following constitutive relations shall be available.

3.3.1 Pressure- and temperature-dependent water properties

3.3.1.1 Introduction

In the governing equations described above (Eqns. (1), (3), (4), (5), and (6)), physical properties such as the density, enthalpy, and viscosity can be strong functions of pressure (P) and temperature (T) making the governing equations very nonlinear. Rational-function approximations (Zyvoloski and Dash 1991b) shall be used to estimate the thermodynamic variables in FEHM over the ranges $0.001 \leq P \leq 110.0$ MPa and $0.001 \leq T \leq 360^\circ\text{C}$. In addition, a second set of rational-function approximations shall be provided for low pressures to give better estimates of the thermodynamic variables over the ranges $0.001 \leq P \leq 20.0$ MPa and $0.5 \leq T \leq 360^\circ\text{C}$.

3.3.1.2 Inputs

The required inputs shall be pressure and temperature at each node at each time step.

3.3.1.3 Processing

The processing shall compute the water properties and their derivatives, using the rational-function approximations, as a function of pressure and temperature at each node at each time step.

3.3.1.4 Outputs

The outputs shall be water density, enthalpy, and viscosity (and their derivatives) at each node at each time step.

3.3.2 Properties of air and air/water vapor mixtures

3.3.2.1 Introduction

The flow of air and air/water vapor mixtures in the porous media shall also be modeled. Appropriate thermodynamic information (density, enthalpy, viscosity, mass fractions) for air and air/water vapor mixtures shall be provided.

3.3.2.2 Inputs

The required inputs will be pressure, temperature, and air/vapor/liquid mass fractions at each node at each time step.

3.3.2.3 Processing

The processing will compute the air and mixture properties at each node at each time step.

3.3.2.4 Outputs

The outputs shall be air and mixture properties (densities, enthalpies, and viscosities) at each node at each time step.

3.3.3 Equation-of-state models

3.3.3.1 Introduction

The ability to use liquids other than water and to use gases other than air in the porous media model shall be provided. The use of equation-of-state models with user-defined parameters allows the introduction of alternate fluids, ideal gases, etc. The models can also be used to provide simplified state relations for water and air.

3.3.3.2 Inputs

The required inputs shall be liquid and vapor reference pressure, temperature, density, enthalpy, and viscosity and their derivatives with respect to temperature and pressure at the reference conditions.

3.3.3.3 Processing

The processing shall compute the fluid properties based on equation-of-state data at each node at each time step.

3.3.3.4 Outputs

The outputs shall be fluid properties (densities, enthalpies, and viscosities) at each node at each time step.

3.3.4 Relative-permeability and capillary-pressure functions

3.3.4.1 Introduction

Relative permeabilities and capillary pressures can be strong functions of saturation. Several well-known relative-permeability functions shall be made available to the user. These functions are the simple linear functions, the Corey (1954) relationships, and the van Genuchten (1980) functions. Composite relative-permeability curves, as described by Klavetter and Peters (1986), shall also be a user option. The capillary functions considered are the linear function and the van Genuchten (1980) capillary-pressure model.

3.3.4.2 Inputs

The required inputs are saturations, pressures, and model parameters implied by the constitutive model to be used.

3.3.4.3 Processing

The processing shall compute relative permeabilities and capillary pressures based on the selected constitutive model.

3.3.4.4 Outputs

The outputs shall be relative permeabilities and capillary pressures at each node.

3.3.5 Adsorbing solutes

3.3.5.1 Introduction

FEHM shall have provisions for adsorbing solutes. The general equilibrium model for adsorption of species onto the reservoir rock is given by (Polzer et al. 1992):

$$C_R = \frac{\alpha_1 C_l^\beta}{1 + \alpha_2 C_l^\beta} \quad (7)$$

The parameters α_1 , α_2 , and β are associated with the sorption models.

3.3.5.2 Inputs

The required inputs shall be all property and parameter values implied by Eqn. (7): concentrations and sorption parameters.

3.3.5.3 Processing

The processing will compute adsorption based on the appropriate model and compute the modified coefficients of the tracer transport equation that account for adsorption reactions.

3.3.5.4 Outputs

The outputs shall be equation coefficients for the finite-element formulation of the tracer transport equations at each node modified to account for adsorption reactions.

3.3.6 Multiple, interacting solutes

3.3.6.1 Introduction

FEHM shall have provisions for multiple, interacting solutes in which chemical reactions involving one or more components are specified. Any number of reactions may be specified with the following form:

$$a_1 S_1 + a_2 S_2 + \dots + a_m S_m = \\ a_{m+1} S_{m+1} + a_{m+2} S_{m+2} + \dots + a_n S_n, \quad (8)$$

where the a 's are the stoichiometric coefficients and the S 's denote each solute present in a particular reaction. This relationship is formulated for each reaction being modeled, and

a solute may be present in any number of reactions as either a reactant or a product.

The rate law governing each reversible reaction shall be specified as follows:

$$\frac{\partial}{\partial t}[S_j] = \pm a_j \left\{ k_{for} \prod_{i=1}^m [S_i]^{b(i)} - k_{rev} \prod_{i=m+1}^n [S_i]^{b(i)} \right\}, \quad (9)$$

where the square brackets [] denote concentration, the $b(i)$ are exponents in the reaction rate equation (specified for every reactant in each reaction), and the forward and reverse reaction rate constants, k_{for} and k_{rev} , are governed by the Arrhenius equation. An option shall be provided to allow or disallow chemical reaction for solute residing on the rock for the case of a sorbing component. Finally, an input option shall be developed so that the user may specify an equilibrium constant for the chemical reaction with the code generating the rate constants k_{for} and k_{rev} such that equilibrium is attained at each time step.

3.3.6.2 Inputs

The required inputs are all property and parameter values implied by Eqns. (8) and (9): concentrations and chemical-reaction model parameters.

3.3.6.3 Processing

The processing shall compute the chemical-reaction source/sink term for each solute.

3.3.6.4 Outputs

The outputs shall be equation coefficients for the finite-element formulation of the tracer transport equations at each node modified to account for chemical reactions.

3.3.7 Dual-porosity formulation

3.3.7.1 Introduction

Many porous-medium problems are dominated by fracture flow. In these cases, the fracture permeability controls the pressure communication in the reservoir even though local storage around the fracture may be dominated by the porous rock, which communicates only with the closest fractures.

Computationally, a volume fraction and length scale shall be used to create one-dimensional versions of Eqns. (3), (4), (5), and (6). The length scale shall be used to modify spatial difference terms, and the volume factors shall be used to modify the

accumulation terms. The volume fractions for the dual-porosity formulation shall satisfy the following relationship:

$$V_f + V_{f1} + V_{f2} = 1 , \quad (10)$$

where V_f is the volume fraction of fractures, V_{f1} is the fraction of the first matrix volume, and V_{f2} is the fraction of the second matrix volume. Note that two nodes shall be used to model the porous rock (matrix). The length scales shall be given by

$$\begin{aligned} L_f &= L_{f0} V_f \\ L_{f1} &= L_{f0} V_{f1} \\ L_{f2} &= L_{f0} V_{f2} \end{aligned} \quad (11)$$

where L_f is the length scale for the fracture volume, L_{f1} is the length scale of the first matrix volume, L_{f2} is the length scale of the second matrix volume, and L_{f0} is a characteristic length scale.

3.3.7.2 Inputs

The required inputs shall be:

- volume fraction of the fracture (V_f) and matrix volumes (V_{f1} , V_{f2}) and
- characteristic length scale for fracture spacing (L_{f0}).

3.3.7.3 Processing

The processing shall modify the equation coefficients (from the finite-element formulation of Eqns. (3), (4), (5), and (6)) at each node using the volume fractions and length scales.

3.3.7.4 Outputs

The outputs shall be the modified equation coefficients at each dual-porosity node.

3.3.8 Double-porosity/double-permeability formulation

3.3.8.1 Introduction

In a partially saturated porous medium, flow is often dominated by capillary suction. In a medium comprised of fractures and matrix, the matrix material has the highest capillary suction, and under relatively static conditions, the moisture resides in the matrix material. Infiltration events, such as severe rainfall, can saturate the porous medium allowing rapid flow in the fractures. To capture this flow phenomena, a system of equations allowing communication between the fractures and

matrix blocks in the reservoir, in addition to the flow within the fractures and matrix blocks, is necessary.

A volume fraction and length scale (different from the dual-porosity formulation) shall be used to characterize the system. Equations (3), (4), (5), and (6) are formulated for both the fracture and matrix computational grids. One-dimensional versions are created to couple locally the two sets of equations. As in the dual-porosity formulation, matrix material communicates only with the local fractures.

The volume fractions for the double-porosity/double-permeability formulation shall satisfy the following relationship:

$$V_f + V_{f1} = 1 , \quad (12)$$

where V_f is the volume fraction of fractures and V_{f1} is the fraction of the matrix volume. The length scales shall be partitioned for the fracture and matrix volumes using

$$\begin{aligned} L_f &= L_{f0} V_f \\ L_{f1} &= L_{f0} V_{f1} \end{aligned} , \quad (13)$$

where L_f is the length scale for the fracture volume, L_{f1} is the length scale of the matrix volume, and L_{f0} is a characteristic length scale.

3.3.8.2 Inputs

The required inputs shall be:

- volume fraction of the fracture (V_f) and
- characteristic length scale for fracture spacing (L_{f0}).

3.3.8.3 Processing

The processing shall modify the equation coefficients (from the finite-element formulation of Eqns. (3), (4), (5), and (6)) at each node using the volume fractions and length scales.

3.3.8.4 Outputs

The outputs shall be the modified equation coefficients at each double-porosity/double-permeability node.

3.3.9 Stress-dependent properties

3.3.9.1 Introduction

Often, it is necessary to accommodate changes in the rock porosity and permeability due to changes in effective stress caused by temperature and pore-fluid pressure changes. A

linear and nonlinear model shall be incorporated in the code for this purpose.

The linear pore-pressure model for porosity is given by

$$\phi = \phi_0 + (1 - \phi_0)(c_r - c_g)(P - P_0) , \quad (14)$$

where ϕ is the porosity at pressure P , ϕ_0 is the porosity at pressure P_0 , c_r is the pore volume compressibility of the rock, and c_g is the compressibility of the matrix grain material.

The nonlinear model for porosity (Gangi 1978) is given by

$$\phi = \phi_0 \left[1 - \left(\frac{P_c}{P_x} \right)^m \right] \quad (15)$$

and

$$P_c = \sigma - P - \alpha E \Delta T , \quad (16)$$

where P_c is the closure stress, σ is the *in situ* stress (assumed isotropic), α is the coefficient of thermal expansion of the rock, E is Young's modulus, ΔT is the temperature change of the rock, and P_x and m are parameters in the model.

For either case, the effect of stress and temperature changes on permeability shall be modeled with

$$k = k_0 \left(\frac{\phi}{\phi_0} \right)^3 , \quad (17)$$

where k is the permeability at porosity ϕ .

3.3.9.2 Inputs

The required inputs shall be the parameters of the appropriate pressure- and temperature-dependent matrix-properties model: pressure, porosity, compressibility, closure stress, *in situ* stress, coefficient of thermal expansion of the rock, Young's modulus, temperature change of the rock, and permeability.

3.3.9.3 Processing

The processing shall compute the fracture and matrix property values using the appropriate pressure- and temperature-dependent matrix-properties model at each node for porous-media, dual-porosity, or double-porosity/double-permeability formulations.

3.3.9.4 Outputs

The outputs shall be the porosity and permeability of each matrix cell.

3.3.10 Variable thermal conductivity

3.3.10.1 Introduction

The thermal conductivity of the solid is often more accurately characterized as a function of temperature or liquid saturation. A linear temperature-dependent model and a relation based upon the square root of liquid saturation shall be incorporated in the code for this reason.

The linear temperature-dependent model is given by

$$K_T = K_{ref} + K_s(T - T_{ref}) , \quad (18)$$

where K_T is the temperature-dependent thermal conductivity, K_{ref} is the thermal conductivity at the reference temperature T_{ref} , and K_s is the slope of the linear relation.

The saturation-dependent thermal-conductivity model is given by

$$K_{sat} = K_{dry} + K_{s,s}\sqrt{S} , \quad (19)$$

where K_{sat} is the saturation-dependent thermal conductivity, K_{dry} is the conductivity at zero saturation, and $K_{s,s}$ is the slope of the linear relationship. Note that the conductivity at complete saturation is $K_{dry} + K_{s,s}$.

3.3.10.2 Inputs

The required inputs shall be the parameters of the appropriate saturation or temperature-dependent thermal conductivity model: temperature, liquid saturation, and the parameters in the above equations.

3.3.10.3 Processing

The processing shall compute the thermal conductivity based on the above relations.

3.3.10.4 Outputs

The output shall be the rock thermal conductivity at each cell.

3.4 Compute Solution to Transient Equations

3.4.1 Implement time-step mechanism

3.4.1.1 Introduction

Transient finite-element solutions proceed forward in time, computing the solution at each time step. A mechanism shall be implemented in which the user can control the initial size of the time step, the maximum allowable time step, and the rate of increase of the time step from one time to the next. This mechanism shall also allow the user to reinitialize the time step, if desired, during the simulation (e.g., a pressure at a source/sink changes dramatically and increased detail is desired or needed for convergence). The time-step mechanism shall also be developed so that the time step is automatically reduced if the solution at a time step does not converge within a specified number of iterations.

3.4.1.2 Inputs

The required inputs shall be:

- the initial time-step size;
- the minimum and maximum time-step values;
- the multiplication factor for increasing the size of the time step;
- a data structure specifying when to set the time step to a new value, what that value is, and what to use for a new multiplication factor;
- the maximum number of iterations to be taken within a time step before the time step is reduced; and
- the maximum number of iterations to be taken for the solution of the total problem.

3.4.1.3 Processing

The processing shall determine the new time step after convergence is achieved for the solution at the current time, and this time step will be added to the current time to obtain the new time. The time step shall not be increased above the maximum specified value. If convergence is not achieved, the time step will be reduced and the step repeated. The time step shall not be reduced below the minimum time-step value.

3.4.1.4 Outputs

The outputs shall be the new time step, the new time, and the number of iterations used to achieve convergence. If the time step has been reduced to the minimum time-step value and convergence is not achieved or the maximum number of

iterations for the total problem has been reached and convergence is not achieved, an error message shall be issued and the program shall exit.

3.4.2 Solve nonlinear equation set at each time step

3.4.2.1 Introduction

In general, the result of the finite-element formulation (Zienkiewicz 1977) of the transient problem shall be a set of nonlinear algebraic equations with unknown values such as pressure, temperature, and concentration that shall be solved at each time step. The equations shall be solved with a Newton-Raphson iterative-solution scheme.

3.4.2.2 Inputs

The required inputs shall be:

- the residual equation for each unknown;
- the derivative of each residual with respect to each unknown; and
- the convergence criterion for solving the system of equations.

3.4.2.3 Processing

The processing shall iteratively determine the pressure/temperature/concentration (solute or air) field by solving the nonlinear equation set using the Newton-Raphson technique until a solution is obtained to the desired degree of accuracy. At each iteration, the system of linear algebraic equations shall be solved using the GZSOLVE application (Zyvoloski and Robinson 1995).

For simulations involving solute transport, it shall be possible to disable the heat and mass portion of the solution and just solve the solute-transport equations.

3.4.2.4 Outputs

The outputs shall be the pressure/temperature/concentration field at the new time.

3.5 Provide Input/Output Data Files

3.5.1 Introduction

All input necessary to perform the finite-element simulation of the model shall be read from one or more input data files. The input data shall be organized in groups of related parameters. The information produced by the program shall be written to one or more output data files so that it may be read by programs using the data, such as plotting or data-analysis routines.

3.5.2 Inputs

The required inputs shall be:

- the finite-element mesh data;
- the initial pressures, temperatures, saturations, and concentrations (solute or gas) within the model domain;
- rock property values within the model domain (conductivity, heat capacity, density);
- data used to set heat- and mass-source/sink strength or pressure;
- data used to set concentration (solute or gas) source strength;
- properties of the finite-element mesh representing the matrix (porosity, permeability);
- finite-element parameters used to control the accuracy of the solution, such as the initial and maximum time steps, the time-step multiplication factor, and convergence criterion; and
- model parameters for selected constitutive relations.

3.5.3 Processing

The processing shall read in all parameter values and generate the finite-element solution to the model. It shall also write the solution to output data files.

3.5.4 Outputs

The outputs shall be:

- pressure, temperature, concentration, and flow field at selected intervals and final time;
- geometric information needed to view the pressure, temperature, concentration, or flow field (i.e., coordinate locations for all nodes); and
- time-varying values of the pressures, temperatures, concentrations, and flow rates of each source/sink or specified matrix location.

3.6 Provide Restart Capability

In large-scale transient simulations, it is often desirable to resume a computation starting at the final time of a previous run or to start with a previously established flow field. This procedure may be done to verify that the run is progressing as desired, to establish a steady-state flow field for a subsequent solute simulation, or to allow modification or inclusion of source/sink conditions starting at this time. The FEHM application shall provide this capability.

3.6.1 Write information needed for restart to output file

3.6.1.1 Introduction

All information needed to resume the computation at the final time of a simulation must first be written to an output file.

3.6.1.2 Inputs

The data needed in a subsequent restart are

- final time of simulation and
- the pressures, temperatures, saturations, and concentrations (solute or noncondensable gas) at the final time step.

3.6.1.3 Processing

The processing shall write all needed data to the output restart file.

3.6.1.4 Outputs

The output shall be a restart file that can be subsequently read to restart a previous simulation or to start a new simulation with an established pressure, temperature, saturation, or concentration field.

3.6.2 Read information needed for restart from restart file

3.6.2.1 Introduction

The information needed to resume the simulation or start a new simulation with an existing pressure and temperature field shall be read in from the restart and primary input files.

3.6.2.2 Inputs

The required inputs are data needed in the restart, including all information written to the restart file in the previous simulation and new information such as source/sink flow rates or pressures for the restart found in the primary input files.

3.6.2.3 Processing

The processing shall read all data from the input files.

3.6.2.4 Outputs

The output shall be a data structure appropriate for resuming the computations, beginning at the final time and the conditions of the previous simulation.

3.6.3 Resume the calculation

3.6.3.1 Introduction

When all input information is read in, the calculation shall resume.

3.6.3.2 Inputs

The required inputs are all input parameter values from the restart and primary input files.

3.6.3.3 Processing

The processing shall perform the calculations as it would in the case of a starting time of 0 with the following exceptions:

- set the start time based on the value from the restart file, rather than 0;
- set the pressure field based on values from the restart file, rather than from the initial pressures;
- set the temperature field based on values from the restart file, rather than from the initial temperatures;
- set the saturations based on values from the restart file; and
- set the concentrations (solute or noncondensable gas) based on values from the restart file.

3.6.3.4 Outputs

The outputs shall be the computational results of a simulation starting at the time and conditions reached at the end of the previous execution of the program.

4.0 EXTERNAL INTERFACE REQUIREMENTS

4.1 User Interfaces

The names of input and output data files used by the programs shall be input interactively at the terminal when the programs are executed or shall be provided in optional configuration data files. All other user interfaces with the programs comprising the FEHM application shall be in the form of ASCII or binary data files. The data files employed by the application are

- an optional configuration data file specifying the names of input and output data files used by each program of the application;
- one or more input data files containing the finite-element mesh information;
- one or more input data files that specify the control parameters, physical parameters, and the source/sink specifications for the model simulation;
- one or more output data files containing the results of the model simulation; and
- a restart data file that contains the information needed to resume a model computation at the termination time of a previous simulation (it becomes an input data file during the restart run).

4.2 Hardware Interfaces

N/A

4.3 Software Interfaces

4.3.1 Linear equation solver

In finite-element simulations, a set of residual equations is usually solved at each time step. When the equations are nonlinear, as in the FEHM

application, the procedure normally employed is iterative, in which a set of linear algebraic equations is solved at each iteration until convergence of the nonlinear equations is achieved. In the FEHM application, the linear equation set at each iteration shall be solved with a reuse component, GZSOLVE, that provides a robust solution method for sparse systems of equations. The FEHM application shall supply the solver with the matrix equation set in a form suitable for the solver, and the solver shall return the solution vector for that iteration.

4.4 Communications Interfaces

N/A

5.0 PERFORMANCE REQUIREMENTS

N/A

6.0 DESIGN CONSTRAINTS

6.1 Standards Compliance

N/A

6.2 Hardware Limitations

N/A

7.0 SECURITY

N/A

8.0 OTHER REQUIREMENTS

8.1 Data Base

N/A

8.2 Operations

N/A

9.0 VALIDATION CRITERIA

Validation criteria shall be developed in Chapter III, "Verification and Validation Plan," of this report.

Chapter II: Software Design

1.0 PURPOSE

In this chapter, the FEHM software is described, including functional requirements, input/output files and their associated variables, and error and warning conditions with their associated messages.

2.0 FUNCTIONAL DESCRIPTION

After a user formulates a problem to be modeled, a mesh representing the physical media is generated. It should be noted that mesh generation is not a primary function of the FEHM application and auxiliary mesh-generation programs are generally used to obtain this input. Data describing the mesh and physical properties of the media and the fluid/gas system to be modeled are input. The appropriate finite-element equations are formulated and constitutive relationships applied. The solution is then computed, and results and restart data are output.

3.0 ASSUMPTIONS AND LIMITATIONS

The assumptions and limitations inherent in FEHM can be categorized as follows:

- The validity of the underlying partial differential equations used to describe the physics of the coupled processes of heat and mass flow in a porous media (see Zyvoloski et al. 1997a). This limitation includes the difficulty in obtaining appropriate input parameters to model given experimental and field data.
- The validity of the computer code used to solve the partial differential equations that describe the physics of flow. This assumption is described further in the last two chapters: "Verification and Validation Plan" and "Verification and Validation Report."
- The ability of the computer code to obtain the advertised performance. This limitation is both machine dependent and user dependent. FEHM is state of the art in both numerical performance and memory management. The numerical performance allows very large (100,000-node) 3-D problems to be run in a workstation environment. Thus, the numerical accuracy needed for typically fine-resolution problems such as contaminant transport can be realized. The memory management allows many jobs to be run on a single workstation and allows quick analysis of problem sensitivities. In our experience, the largest source of poor code performance, both in accuracy and CPU speed, is user error. FEHM is a complicated tool and requires a high level of user experience in simulation and groundwater applications. The FEHM "User's Manual" and other documents (Zyvoloski et al. 1997b) are updated regularly with major input from users.

4.0 PRIMARY PRODUCT DESCRIPTIONS

The FEHM application consists of one primary product, program **fehm**, which is used to formulate a transient problem that generates a set of nonlinear algebraic equations. The nonlinear equations are solved using the GZSOLVE application (Zyvoloski and Robinson 1995).

4.1 FEHM

4.1.1 Purpose

See Section 1.0 of this chapter.

The functional requirements satisfied by the **fehm** program are summarized in Table 1, where the section numbers refer to the previous chapter, "Software Requirements Specification."

Table 1. Functional requirements of the FEHM application		
Requirement	Section	Implemented by
Finite-element coefficient generation	3.1	anonp, area2d_tri, check_sx, determ, gencof, gncf2, gncf3, mdnodes, pebi, pebi3, radius, setzone, sfn2r, sfn3r, shap2r, shap3p, shap3r, split, sx_combine, thickness
Formulate transient equations	3.2	
Heat-conduction equations	3.2.1	bnsver, geneq3, gensl3
Heat- and mass-transfer equations	3.2.2	air_rdof, airctr, bnsver, co2ctr, dpdp3, dpdpfa, dpdpfh, dualax, dualfa, dualfh, geneq1, geneq2, geneqc, geneqmdnode, gensdp, gensdp3, gensl1, gensl2, gensl4, interblock_iso, mod_eqs_ngas, thermw, thrair, thrmw, varchk, zeolites
Noncondensable-gas flow equations	3.2.3	air_rdof, airctr, bnsver, co2ctr, dualfa, geneq2, geneqc, geneqmdnode, gensdp, gensl2, gensl4, interblock_iso, thrair, thrmw, varchk
Solute-transport equations	3.2.4	angle3, cnsver, concadiff, concen, coneq1, coneq1mdnode, csolve, dpdpfa, dualta, dualtx, eullag3, gencon, gentdp, node_rxn, react, rotate, solstore, thermc, varchk
Particle-tracking module	3.2.5	cell_time, getconc, inptrk, inverf, part_track, set_ptrk, time_diff, time_disp2, wrtptrk
Sources and sinks	3.2.6	bcon, inflo2, inflow, inhflx, thermw, thermc, thrair, thrmw, zeolites
Apply constitutive relationships	3.3	
Pressure- and temperature-dependent water properties	3.3.1	data, enthp, outbnd, psat, psatl, thermw, thrmw, thrair, varchk
Properties of air and air/water vapor mixtures	3.3.2	air_cp, dvacalc, outbnd, psatl, thrair, thrmw, vaporl, varchk
Equation-of-state models	3.3.3	coeffc, sther, varchk
Relative-permeability and capillary-pressure functions	3.3.4	cappr, rlperm, vgcap, vgcap_fit, vgrlp
Adsorbing solutes	3.3.5	mult_rxn, rdcon, read_rxn, solstore, thermc
Multiple, interacting solutes	3.3.6	mult_rxn, node_rxn, react, read_rxn, rxn_product, setup_rxn, thermc

Table 1. Functional requirements of the FEHM application (continued)		
Requirement	Section	Implemented by
Dual-porosity formulation	3.3.7	dual, duallex, dualfa, dualfh, dualta, dualtx
Double-porosity/double-permeability formulation	3.3.8	crdpdp, ctdpdp, dpdp, dpdp3, dpdpfa, dpdpfh, dpdpta, indpdp, rddpdp
Stress-dependent properties	3.3.9	porosi, vfcal
Variable thermal conductivity	3.3.10	vcon
Compute solution to transient equations	3.4	
Implement time-step mechanism	3.4.1	csolve, daycrl, fehmn, intime, resetttrc, resetv, timcrl
Solve nonlinear equation set at each time step	3.4.2	bnsver, cnswer, gencon, gensdp, gensdp3, gensl1, gensl2, gensl3, gensl4, gentdp, mod_eqs_ngas, normal, normal_dof, nrmlz4, rd1dof, rdof_new, setord, solve, switch, switchb, and GZSOLVE application (Zyvoloski and Robinson 1995)
Provide input/output data files	3.5	
		avs_io, cntlin, cntlio, done_macro, file_prefix, infile, iofile, namefile2, setunits, start_macro, termin, termio, writeio
Inputs	3.5.2	airctr, co2ctr, concen, disk, diskc, diskp, dpdp, dual, flxo, gendat, geoin, incond, incoord, inctrl, inflo2, inflow, inhflx, initdata, inmentat, innode, inpatran, inperm, inpres, inptrk, input, inrock, intime, inzeol, mdnodes, porosi, rdcon, rddpdp, rdthick, read_avs_io, read_rxn, read_sx, renum, rlperm, scanin, setparams, sice, sther, storsx, user, vcon, welbor, zone
Outputs	3.5.4	avs_write_cord, avs_write_struc, contr, contrc, contrj, datchk, diagnostics, disk, diskc, diskp, elem_type, elem_type_binary, flxo, input, outbnd, plot, plotc1, storsx, write_avs_node_con, write_avs_node_mat, write_avs_node_s, write_avs_node_v, write_avs_ucl_header, write_binary_geo, write_binary_header, write_binary_node_con, write_binary_node_mat, write_binary_node_s, write_binary_node_v, wrtcon, wrtout, wrtptrk, zone
Provide restart capability	3.6	
Write information needed for a restart to an output file	3.6.1	disk, diskc, diskp, timcrl
Read information needed for a restart from a restart file	3.6.2	disk, diskc, diskp, startup
Resume the calculation	3.6.3	concen, fehmn, startup

4.1.2 Functional description

See Section 2.0 of this chapter.

A simplified flow chart illustrating the segmentation of the application is provided in the FEHM document "Summary of Models and Methods" (Zyvoloski et al 1997a). A summary listing of the subroutines and functions invoked by the **fehm** program is given in Appendix A of this report.

4.1.3 Assumptions and limitations

See Section 3.0 of this chapter.

4.1.4 Input/output

4.1.4.1 Configuration interface table

N/A

4.1.4.2 Other input data files

4.1.4.2.1 Input control file. The input control file provides the **fehm** program with the names of input/output (I/O) files to be used by the program, the terminal output control flag, and the user subroutine number (Table 2). Names for the files, which may include subdirectories or paths, are entered one per line followed by the terminal output control flag and user subroutine number. A blank line may be entered for any item not required by the user. Variable *nmfil(1)* contains the name of the input control file. The default control file name is *fehmn.files*.

Table 2. Input control file		
Input variable	Format	Description
<i>nmfil(2)</i>	character*100	Main input file name
<i>nmfil(3)</i>	character*100	Geometry-data input file name
<i>nmfil(4)</i>	character*100	Zone-data input file name
<i>nmfil(5)</i>	character*100	Main output file name
<i>nmfil(6)</i>	character*100	Restart input file name
<i>nmfil(7)</i>	character*100	Restart output file name
<i>nmfil(8)</i>	character*100	Simulation-history output file name
<i>nmfil(9)</i>	character*100	Solute-history output file name
<i>nmfil(10)</i>	character*100	Contour-plot output file name
<i>nmfil(11)</i>	character*100	Dual-porosity or double-porosity/double-permeability contour plot output file name
<i>nmfil(12)</i>	character*100	Coefficient-storage file name
<i>nmfil(13)</i>	character*100	Input-check output file name

Table 2. Input control file (continued)		
Input variable	Format	Description
<i>tty_flag</i>	character*4	Terminal output flag: all, some, none
<i>usub_num</i>	integer	User subroutine call number

4.1.4.2.2 Main input data file. The main input file contains user parameter initialization values and problem control information (Table 3). The default input data file name is *fehmn.dat*.

Table 3. Main input data file		
Input variable	Format	Description
<i>wdd</i>	character*80	Title line.
<i>macro</i>	character*4	Any macro keyword described below, except coor and elem , may use <i>lockkeyword</i> and <i>locfilename</i> to designate that the regular data should be read from an auxiliary input file.
<i>lockkeyword</i>	character*4	Keyword " file " to designate that an auxiliary input file is used.
<i>locfilename</i>	character*100	Name of the optional data input file.
<i>macro</i>	character*4	Keyword " adif " (optional).
<i>tort</i>	real	Tortuosity for air-water vapor diffusion.
<i>macro</i>	character*4	Keyword " airwater " (optional).
<i>ico2d</i>	integer	Type of air module to use.
<i>tref</i>	real	Reference temperature for properties (°C).
<i>pref</i>	real	Reference pressure for properties (MPa).
<i>macro</i>	character*4	Keyword " alti " (not supported this version).
<i>macro</i>	character*4	Keyword " boun " (optional)
<i>keyword</i>	character*4	Keyword specifying a model designation, time for boundary condition or source changes, or actual variable or source change. Keywords are: model - new model definition to follow. ti - time sequence for changes to follow. cy - cyclic time sequence for changes to follow. sa - air-source sequence for changes to follow. sw - water-source sequence for changes to follow. se - enthalpy-source sequence for changes to follow. dsa - distributed air-source sequence for changes to follow. dsw - distributed water-source sequence for changes to follow. dse - distributed enthalpy-source sequence for changes to follow. s - fixed saturation sequence for changes to follow. hd - fixed hydraulic-head sequence for changes to follow. pw - fixed water-pressure sequence for changes to follow. pa - fixed air-pressure sequence for changes to follow. pwo - fixed water-pressure sequence for changes to follow (constrained to outflow only). pao - fixed air-pressure sequence for changes to follow (constrained to outflow only).

Table 3. Main input data file (continued)

Input variable	Format	Description
		en - fixed enthalpy-sequence for changes to follow. t - fixed temperature-sequence for changes to follow. h - fixed humidity-sequence for changes to follow (must be used with van Genuchten relative-permeability model). ft - fixed flowing-temperature-sequence for change to follow. By flowing temperature, we mean the temperature of the inflow stream for a specified source. If no influx source occurs where this condition is applied, it will be ignored. if - impedance factor for use with fixed water-pressure boundary condition. If left out, the impedance factor will be set to the volume of the grid cell. ts - timestep sequence for changes to follow. end - signifies end of keyword input (a blank line will also work). NOTE: Either KEYWORD 'ti' or 'cy' must be the first KEYWORD after a new model (KEYWORD 'model') is started.
<i>ntimes</i>		Number of time changes for boundary condition or source specification. This parameter is only associated with KEYWORDS 'ti' and 'cy', i.e., those that are associated with time sequences.
<i>time_model</i>		Times for changes in boundary conditions or sources.
<i>variable_model</i>		New values for boundary conditions or sources.
<i>ja</i>	integer	First node to be assigned properties. If <i>ja</i> < 0, the zone to be assigned properties.
<i>jb</i>	integer	Last node to be assigned properties.
<i>jc</i>	integer	Loop increment for assigning properties.
<i>model_number</i>	integer	Number referring to the numerical order in which the models were input (begin with KEYWORD 'model').
A blank line to signal end of boundary condition input.		
<i>macro</i>	character*4	Keyword " bous " (optional).
<i>ibous</i>	real	To enable constant density and viscosity for the flow terms (Boussinesq-type approximation), <i>ibous</i> = 1.
<i>macro</i>	character*4	Keyword " cond " (required).
<i>ja, jb, jc</i>	integer	See description above under keyword " boun ".
<i>thxd</i>	real	Thermal conductivities in the x-direction, y-direction, and z-direction
<i>thyd</i>	real	($\frac{W}{m \cdot K}$).
<i>thzd</i>	real	
A blank line to signal end of conductivity input.		
<i>macro</i>	character*4	Keyword " cont " (optional).
<i>ncntr</i>	integer	Time-step interval for contour plots (number of time steps).
<i>contim</i>	real	Time interval for contour plots (days).
or		
<i>altc</i>	character*4	Keyword specifying the type of contour output wanted: "avs", "fehm", "free", "ment", "ptrn".
<i>ncntr</i>	integer	Same as above.
<i>contim</i>	real	Same as above.

Table 3. Main input data file (continued)

Input variable	Format	Description
<i>chdum</i>	character*72	Keyword used when <i>altc</i> is "avs" specifying type of contour-plot data files to be created. Valid keywords (case insensitive) are: (m)aterial - output contour values for material properties. (l)iquid - output contour values for liquid phase. (v)aapor - output contour values for vapor phase. (v)e)locity - output velocity values. (dp)dp - output contour values for dual-permeability nodes. (p)ressure - output pressure values. (t)emperature - output temperature values. (s)aturation - output saturation values. (c)oncentration - output solute concentration values. (f)ormatted - output data in ASCII format. (u)nformatted - output data in binary format. (e)ndavs - last keyword entered. Keywords are entered one per line, and the letters given in () are sufficient to identify the keyword.
<i>macro</i>	character*4	Keyword " coor " (required). See Section 4.1.4.2.3 on page 49.
<i>macro</i>	character*4	Keyword " ctrl " (required).
<i>maxit</i>	integer	Maximum number of iterations allowed in either the overall Newton cycle or the inner cycle to solve for the corrections at each iteration.
<i>epm</i>	real	Tolerance for Newton cycle (nonlinear-equation tolerance).
<i>north</i>	integer	Number of orthogonalizations in the linear equation solver.
<i>ja, jb, jc</i>	integer	See description under keyword " boun " (page 37).
<i>igauss</i>	integer	The order of partial Gauss elimination. Larger values increase memory use but may be necessary for convergence.
A blank line to signal end of Gauss elimination order input.		
<i>aaw</i>	real	Implicitness factor.
<i>agrav</i>	integer	Direction of gravity.
<i>upwgt</i>	real	Value of upstream weighting.
<i>iamm</i>	integer	Maximum number of iterations for which the code will multiply the time-step size.
<i>aiaa</i>	real	Time-step multiplier.
<i>daymin</i>	real	Minimum time-step size (days).
<i>daymax</i>	real	Maximum time-step size (days).
<i>icnl</i>	integer	Parameter that specifies the geometry.
<i>lda</i>	integer	Parameter that specifies the external storage of geometric coefficients.
<i>macro</i>	character*4	Keyword " dof " (not implemented).
<i>macro</i>	character*4	Keyword " dpdp " (optional).
<i>idpdp</i>	integer	Solution descriptor for double-porosity/double-permeability solution.
<i>ja, jb, jc</i>	integer	See description under keyword " boun " (page 37).
<i>volfd1</i>	real	Volume fraction for fracture node.
A blank line to signal end of volume-fraction input.		
<i>ja, jb, jc</i>	integer	See description under keyword " boun " (page 37).
<i>apuv1</i>	real	Length scale for matrix nodes (m).
A blank line to signal end of length-scale input.		

Table 3. Main input data file (continued)

Input variable	Format	Description
<i>macro</i>	character*4	Keyword " dual " (optional).
<i>idualp</i>	integer	Solution descriptor for dual-porosity solution.
<i>ja, jb, jc</i>	integer	See description under keyword " boun " (page 37).
<i>vold1</i>	real	Volume fraction for fracture portion of the continuum.
A blank line to signal end of volume fraction for fracture input.		
<i>ja, jb, jc</i>	integer	See description under keyword " boun " (page 37).
<i>vold2</i>	real	Volume fraction for the first matrix portion of the continuum.
A blank line to signal end of volume fraction for matrix input.		
<i>ja, jb, jc</i>	integer	See description under keyword " boun " (page 37).
<i>apuvd</i>	real	Length scale for matrix nodes (m).
A blank line to signal end of length-scale input.		
<i>macro</i>	character*4	Keyword " elem " (required). See Section 4.1.4.2.3 on page 49.
<i>macro</i>	character*4	Keyword " eos " (optional).
<i>ieosd</i>	integer	Equation-of-state reference number.
<i>ipsat</i>	integer	Parameter to set vapor pressure to zero.
<i>itsat</i>	integer	Parameter to adjust the saturation temperature.
<i>ew1</i>	real	Liquid reference pressure (MPa).
<i>ew2</i>	real	Liquid reference temperature (°C).
<i>ew3</i>	real	Liquid reference density (kg/m ³).
<i>ew4</i>	real	Derivative of liquid density with respect to pressure at reference conditions.
<i>ew5</i>	real	Derivative of liquid density with respect to temperature at reference conditions.
<i>ew6</i>	real	Liquid reference enthalpy (MJ/kg).
<i>ew7</i>	real	Derivative of liquid enthalpy with respect to pressure at reference conditions.
<i>ew8</i>	real	Derivative of liquid enthalpy with respect to temperature at reference conditions.
<i>ew9</i>	real	Liquid reference viscosity.
<i>ew10</i>	real	Derivative of liquid viscosity with respect to pressure at reference conditions.
<i>ew11</i>	real	Derivative of liquid viscosity with respect to temperature at reference conditions.
<i>ev1</i>	real	Vapor reference pressure (MPa).
<i>ev2</i>	real	Vapor reference temperature (°C).
<i>ev3</i>	real	Vapor reference density (kg/m ³).
<i>ev4</i>	real	Not used, included only to maintain a similar format to liquid parameters.
<i>ev5</i>	real	Not used, included only to maintain a similar format to liquid parameters.
<i>ev6</i>	real	Vapor reference enthalpy (MJ/kg).
<i>ev7</i>	real	Derivative of vapor enthalpy with respect to pressure at reference conditions.
<i>ev8</i>	real	Derivative of vapor enthalpy with respect to temperature at reference conditions.

Table 3. Main input data file (continued)

Input variable	Format	Description
<i>ev9</i>	real	Vapor reference viscosity.
<i>ev10</i>	real	Derivative of vapor viscosity with respect to pressure at reference conditions.
<i>ev11</i>	real	Derivative of vapor viscosity with respect to temperature at reference conditions.
<i>macro</i>	character*4	Keyword " exrl " (optional)
<i>iexrlp</i>	integer	To enable explicit relative permeability, <i>iexrlp</i> = 1.
<i>macro</i>	character*4	Keyword " finv " (optional; no input is associated with this macro).
<i>macro</i>	character*4	Keyword " flow " (required if flow problem).
<i>ja, jb, jc</i>	integer	See description under keyword " boun " (page 37).
<i>skd</i>	real	Depending on problem type: Heat- and/or mass-source strength (kg/s), heat only (MJ/s); Specified source air pressure (MPa); or Pressure above which outflow occurs (MPa).
<i>eflow</i>	real	Depending on problem type: Enthalpy of fluid injected (MJ/kg); Temperature (°C); Source liquid saturation (kg/s); or Source air pressure (MPa).
<i>aiped</i>	real	Impedance parameter.
A blank line to signal end of flow input.		
<i>macro</i>	character*4	Keyword " flo2 " (optional).
<i>ja, jb, jc, jd</i>	integer	See description under keyword " boun " (page 37).
<i>skd</i>	real	Same as above for keyword " flow ".
<i>eflow</i>	real	Same as above for keyword " flow ".
<i>aiped</i>	real	Same as above for keyword " flow ".
A blank line to signal end of flo2 input.		
<i>macro</i>	character*4	Keyword " flxo " (optional).
<i>nflx</i>	integer	Number of internode fluxes to be calculated.
<i>iflx1</i>	integer	First node to be used in flux calculation.
<i>iflx2</i>	integer	Second node to be used in flux calculation. If <i>iflx2</i> = 0, then the node connected to <i>iflx1</i> with the greatest internodal distance is used to calculate the mass flux.
<i>x1</i>	real	X-, y-, and z-coordinates of the first node to be used in flux calculation.
<i>y1</i>	real	Used only for those nodes where <i>IFLX1</i> < 0.
<i>z1</i>	real	
<i>x2</i>	real	X-, y-, and z-coordinates of the second node to be used in flux calculation.
<i>y2</i>	real	Used only for those nodes where <i>IFLX2</i> < 0.
<i>z2</i>	real	
<i>macro</i>	character*4	Keyword " head " (optional). (No input is associated with this macro.)
<i>macro</i>	character*4	Keyword " hflx " (optional).
<i>ja, jb, jc</i>	integer	See description under keyword " boun " (page 37).
<i>qflux</i>	real	If <i>qflxm</i> = 0, then <i>qflux</i> is the heat flux (MW). If <i>qflxm</i> ≠ 0, then <i>qflux</i> is a temperature (°C) and the heat flux is calculated according to the formula: $Q_H = qflxm(TL - qflux)$ (MW).
<i>qflxm</i>	real	If <i>qflxm</i> ≠ 0, multiplier for heat-flux equation given in description (MW/°C).
A blank line to signal end of heat-flux input.		

Table 3. Main input data file (continued)

Input variable	Format	Description
<i>macro</i>	character*4	Keyword "ice" (optional).
<i>ice</i>	integer	Solution descriptor for ice solution.
<i>siin</i>	real	Default value for ice saturation.
<i>tmelt</i>	real	Freezing temperature of water (°C).
<i>ja, jb, jc</i>	integer	See description under keyword "boun" (page 37).
<i>sii</i>	real	Ice saturation.
A blank line to signal end of ice-saturation input.		
<i>macro</i>	character*4	Keyword "init" (required if "pres" not used).
<i>pein</i>	real	Initial value of pressure (MPa).
<i>tin</i>	real	Initial value of temperature (°C).
<i>tin1</i>	real	Temperature-gradient linear formula parameter (°C).
<i>grad1</i>	real	Temperature-gradient linear formula parameter (°C/m).
<i>depth</i>	real	Temperature-gradient formula parameter (m).
<i>tin2</i>	real	Temperature-gradient quadratic formula parameter (°C).
<i>grad2</i>	real	Temperature-gradient quadratic formula parameter (°C/m).
<i>quad</i>	real	Temperature-gradient quadratic formula parameter (°C/m ²).
<i>macro</i>	character*4	Keyword "iter" (optional).
<i>g1</i>	real	Multiplier for the linear convergence region of the Newton-Raphson iteration.
<i>g2</i>	real	Multiplier for the quadratic convergence region of the Newton-Raphson iteration.
<i>g3</i>	real	Tolerance for the adaptive implicit method (multiplying factor for Newton-Raphson tolerance).
<i>tmch</i>	real	Machine tolerance. If satisfied by the residual norm, the Newton iteration is assumed to be complete.
<i>overf</i>	real	Over-relaxation factor for passive nodes in adaptive implicit method.
<i>irdof</i>	integer	Enables the reduced degree-of-freedom method.
<i>islord</i>	integer	Reordering parameter.
<i>iback</i>	integer	IRDOF parameter.
<i>icoupl</i>	integer	Number of SOR iterations used in reduced degree-of-freedom methods.
<i>rnmax</i>	real	Maximum running time for problem before the solution is stopped (cpu minutes).
<i>macro</i>	character*4	Keyword "itup" (optional).
<i>iad_up</i>	integer	Number of iterations after which the upwind directions are held constant.
<i>macro</i>	character*4	Keyword "iupk" (optional; no input is associated with this macro).
<i>macro</i>	character*4	Keyword "ivfc" (not supported this version).
<i>macro</i>	character*4	Keyword "mdnode" (optional).
<i>num_md</i>	integer	Number of new connections to be entered.
<i>max_con</i>	integer	Maximum number of new connections to a given node.
<i>ielim</i>	integer	Redundant nodal connections are eliminated as needed if <i>ielm</i> < 0.
<i>sx_mult</i>	real	Multiplier for equilibrium conditions.
For each new connection (<i>num_md</i>):		
<i>node</i>	integer	Node to which new connection is established.
<i>ipar</i>	integer	Not used at present. Its value is ignored but the number entered must be an integer.
<i>npar</i>	integer	The new connected node. If <i>npar</i> = <i>node</i> , no new connection is established.

Table 3. Main input data file (continued)

Input variable	Format	Description
<i>macro</i>	character*4	Keyword " ngas " (optional).
<i>ico2d</i>	integer	Solution descriptor for noncondensable gas transport.
<i>ja, jb, jc</i>	integer	See description under keyword " boun " (page 37).
<i>pco2</i>	real	Initial partial pressure of noncondensable gas. If <i>pco2</i> < 0, then ABS (<i>pco2</i>) is interpreted as a temperature and the partial pressure of the noncondensable gas is calculated.
A blank line to signal end of partial-pressure input.		
<i>ja, jb, jc</i>	integer	See description under keyword " boun " (page 37).
<i>cpnk</i>	real	If <i>cpnk</i> < 0, then ABS (<i>cpnk</i>) is the specified noncondensable pressure and will be held at that value. If <i>cpnk</i> > 0, then <i>cpnk</i> is the specified relative humidity and the saturation is calculated using the vapor-pressure lowering formula and the capillary-pressure formula.
A blank line to signal end of saturation input.		
<i>ja, jb, jc</i>	integer	See description under keyword " boun " (page 37).
<i>qcd</i>	real	Specified air flow rate (kg/s).
A blank line to signal end of air-flow-rate input.		
<i>macro</i>	character*4	Keyword " nod2 " (required if macro node is not used).
<i>m</i>	integer	Number of nodes for which information will be printed to output files.
<i>m2</i>	integer	Number of nodes for short list (terminal printout).
<i>mn(i)</i>	integer	<i>m</i> node numbers for which information will be printed on the output file (<i>i</i> = 1 to <i>m</i>). If a <i>mn(i)</i> < 0, then coordinates are used to define that node.
<i>x, y, z</i>	real	Coordinates of node for which information will be printed. One line for each <i>mn</i> < 0. The code finds the node closest to the coordinate given.
<i>mni(i)</i>	integer	<i>m2</i> node numbers for which information will be printed on the output file (<i>i</i> = 1 to <i>m2</i>). If a <i>mni(i)</i> < 0, then coordinates are used to define that node.
<i>x, y, z</i>	real	Coordinates of node for which information will be printed. One line for each <i>mni</i> < 0. The code finds the node closest to the coordinate given.
<i>macro</i>	character*4	Keyword " node " (required if macro nod2 is not used).
<i>m</i>	integer	Number of nodes for which information will be printed to output files.
<i>mn(i)</i>	integer	<i>m</i> node numbers for which information will be printed on the output file (<i>i</i> = 1 to <i>m</i>). If a <i>mn(i)</i> < 0, then coordinates are used to define that node.
<i>x, y, z</i>	real	Coordinates of node for which information will be printed. One line for each <i>mn</i> < 0. The code finds the node closest to the coordinate given.
or		
<i>keyword</i>	character*5	Keyword " block " to invoke node specification by <i>ja, jb, jc</i> format.
<i>ja, jb, jc</i>	integer	See description under keyword " boun " (page 37).
A blank line to signal end of node-block input.		
<i>macro</i>	character*4	Keyword " num " (not implemented).
<i>macro</i>	character*4	Keyword " perm " (required).
<i>ja, jb, jc</i>	integer	See description under keyword " boun " (page 37).
<i>pnx</i>	real	Permeability in the x-direction (m^2).
<i>pny</i>	real	Permeability in the y-direction (m^2).
<i>pnz</i>	real	Permeability in the z-direction (m^2).
A blank line to signal end of permeability input.		

Table 3. Main input data file (continued)

Input variable	Format	Description
<i>macro</i>	character*4	Keyword " pest " (optional).
<i>mpest</i>	integer	Number of nodes for PEST output (pressures, saturations, temperatures).
<i>npest</i>	integer	Node numbers whose values are printed to output file (suffix .pest).
<i>x, y, z</i>	real	Coordinates of node for which information will be printed. One line for each <i>npest</i> < 0. The code finds the node closest to the coordinate given.
<i>macro</i>	character*4	Keyword " ppor " (optional).
<i>iporos</i>	integer	Porosity/permeability type: <i>iporos</i> = -1, specific storage model; <i>iporos</i> = 1, aquifer compressibility model; and <i>iporos</i> = -2, Gangi model.
<i>ja, jb, jc</i>	integer	See description under keyword " boun " (page 37).
<i>por1</i>	real	Specific storage (<i>iporos</i> = -1), aquifer compressibility (<i>iporos</i> = 1), or Gangi model exponent <i>m</i> (<i>iporos</i> = -2).
<i>por2</i>	real	Gangi model pressure, P_x (MPa).
<i>por3</i>	real	Gangi model in-situ stress, σ (MPa).
<i>por4</i>	real	Gangi model product of the coefficient of thermal expansion for the rock and Young's modules, (αE) (MPa/°C).
A blank line to signal end of ppor model parameter input		
<i>macro</i>	character*4	Keyword " pres " (required if macro init not used).
<i>ja, jb, jc</i>	integer	See description under keyword " boun " (page 37).
<i>phrd</i>	real	Initial pressure (MPa).
<i>tind</i>	real	Initial temperature (°C) or initial saturation depending on thermodynamic region.
<i>ieosd</i>	integer	Thermodynamic-region parameter.
A blank line to signal end of initial-value input.		
<i>macro</i>	character*4	Keyword " ptrk " (optional).
<i>npart</i>	integer	Number of particles in the simulation.
<i>rseed</i>	integer	6-digit integer random-number seed.
<i>daycs</i>	real	Time for which the particle-tracking solution is enabled (days).
<i>daycf</i>	real	Time for which the particle-tracking solution is disabled (days).
<i>dayhf</i>	real	Time for which the flow solution is disabled (days).
<i>dayhs</i>	real	Time for which the flow solution is enabled (days).
<i>trak_type</i>	integer	Flag to denote the fluid phase of the particles.
<i>half_life</i>	real	Half-life for irreversible first-order decay reaction (s).
<i>pout</i>	integer	Flag to specify the concentration output.
<i>prnt_rst</i>	integer	Flag to specify whether particle information is written to the ".fin" file.
<i>transflag</i>	integer	Flag to specify which transport mechanisms apply.
<i>kd</i>	real	Sorption coefficient (linear, reversible, equilibrium sorption) (kg-fluid/kg-rock).
<i>tclx</i>	real	Dispersivity in the x-direction (m).
<i>tcl y</i>	real	Dispersivity in the y-direction (m).
<i>tclz</i>	real	Dispersivity in the z-direction (m).
<i>diffmat</i>	real	Molecular diffusion coefficient in the rock matrix (m ² /s).
<i>rd_frac</i>	real	Retardation factor within the primary porosity (fractures) for a matrix-diffusion particle-tracking simulation.

Table 3. Main input data file (continued)

Input variable	Format	Description
<i>matrix_por</i>	real	Porosity of the rock matrix.
<i>fspacing</i>	real	Mean fracture spacing (m).
<i>ja, jb, jc</i>	integer	See description under keyword "boun" (page 37).
<i>itrc</i>	integer	Model number for parameters defined above.
A blank line to signal end of model-number input.		
<i>ja, jb, jc</i>	integer	See description under keyword "boun" (page 37).
<i>pcnsk</i>	real	Particle-injection parameter.
<i>t1sk</i>	real	Time (days) when particle injection begins.
<i>t2sk</i>	real	Time (days) when particle injection ends.
A blank line to signal end of particle-injection parameter input.		
<i>macro</i>	character*4	Keyword "renm" (optional).
<i>ja, jb, jc</i>	integer	See description under keyword "boun" (page 37).
<i>igd</i>	integer	New node number for given node.
A blank line to signal end of renumbering input.		
<i>macro</i>	character*4	Keyword "rflx" (not implemented in this version of FEHM).
<i>macro</i>	character*4	Keyword "rlp" (optional).
<i>irlp(i)</i>	integer	Relative-permeability model type.
<i>rp1</i>	real	Parameter used in all models. For models 1 and 2, irreducible liquid saturation. For models 3 and 4, residual liquid saturation.
<i>rp2</i>	real	Parameter used in all models. For models 1 and 2, irreducible vapor saturation. For models 3 and 4, maximum liquid saturation.
<i>rp3</i>	real	Parameter used in models 1, 3, and 4. For model 1, maximum liquid saturation. For models 3 and 4, α_G parameter (1/m) (note: some data are given in (1/Pa); convert using pressure = $\rho g \Delta h$).
<i>rp4</i>	real	Parameter used in models 1, 3, and 4. For model 1, maximum vapor saturation. For models 3 and 4, parameter n.
<i>rp5</i>	real	Parameter used in models 3 and 4. Multiple of cutoff capillary pressure assigned as maximum capillary pressure.
<i>rp6</i>	real	Parameter used in models 3 and 4. Cutoff saturation <i>rp1</i> .
<i>rp7</i>	real	Parameter used in model 4. Residual liquid saturation for fracture.
<i>rp8</i>	real	Parameter used in model 4. Maximum liquid saturation for fracture.
<i>rp9</i>	real	Parameter used in model 4. α_G for fractures.
<i>rp10</i>	real	Parameter used in model 4. n for fractures.
<i>rp11</i>	real	Parameter used in model 4. Same as <i>rp5</i> except for fractures.
<i>rp12</i>	real	Parameter used in model 4. Same as <i>rp6</i> except for fractures.
<i>rp13</i>	real	Parameter used in model 4. Fracture intrinsic permeability (m ²).
<i>rp14</i>	real	Parameter used in model 4. Matrix intrinsic permeability (m ²).
<i>rp15</i>	real	Parameter used in model 4. Fracture porosity.
<i>ja, jb, jc</i>	integer	See description under keyword "boun" (page 37).
<i>i</i>	integer	Number referring to the sequence of models read.
A blank line to signal end of relative-permeability model input.		
<i>rlpfile</i>	character*100	Name of the optional rlp data file used when <i>irlp(i)</i> = 5.

Table 3. Main input data file (continued)

Input variable	Format	Description
<i>macro</i>	character*4	Keyword "rock" (required).
<i>ja, jb, jc</i>	integer	See description under keyword "boun" (page 37).
<i>denrd</i>	real	Rock density (kg/m ³).
<i>cprd</i>	real	Rock specific heat ($\frac{\text{MJ}}{\text{kg} \cdot \text{K}}$).
<i>psd</i>	real	Porosity.
A blank line to signal end of rock input.		
<i>macro</i>	character*4	Keyword "rxn" (optional).
<i>key_group</i>	character	Key word to specify that species are to be placed into groups that are solved simultaneously.
<i>ngroups</i>	integer	Number of groups of species.
<i>group</i>	integer	<i>nspecies</i> values are entered for each line of input, and <i>ngroups</i> lines of input are required, one for each group.
<i>nrxns</i>	integer	Number of chemical reactions.
<i>rxn_interval</i>	real	Time between each iteration.
<i>key_rxn</i>	character*4	Denotes the type of reaction. The first letter of the keyword is all that is required.
<i>equil_model</i>	integer	Flag denoting which model is to be used for defining the temperature dependence of the equilibrium constant.
<i>equil_const25</i>	real	The term A_{rxn} in equilibrium constant-temperature-dependence model.
<i>enthalpy25</i>	real	The term ΔH_H in equilibrium constant-temperature-dependence model.
<i>gamma_check</i>	real	Equilibrium-tolerance parameter γ_{tol} .
<i>rate_factor</i>	real	Parameter for scaling the rate constants.
<i>round_tol</i>	real	Cut-off parameter for forward reaction rate.
or		
<i>key_rxn</i>	character*4	Same as above.
<i>equil_model</i>	integer	Same as above.
<i>awwa(1)</i>	real	The term $A_{\text{rxn},1}$ in equilibrium constant-temperature-dependence model.
<i>awwa(2)</i>	real	The term $A_{\text{rxn},2}$ in equilibrium constant-temperature-dependence model.
<i>awwa(3)</i>	real	The term $A_{\text{rxn},3}$ in equilibrium constant-temperature-dependence model.
<i>awwa(4)</i>	real	The term $A_{\text{rxn},4}$ in equilibrium constant-temperature-dependence model.
<i>awwa(5)</i>	real	The term $A_{\text{rxn},5}$ in equilibrium constant-temperature-dependence model.
<i>gamma_check</i>	real	Same as above.
<i>rate_factor</i>	real	Same as above.
<i>round_tol</i>	real	Same as above.
or		
<i>key_rxn</i>	character*4	Same as above.
<i>ar_for</i>	real	Pre-exponential factor of the forward reaction.
<i>ea_for</i>	real	Activation energy of the forward reaction (kJ/mol).
<i>ar_rev</i>	real	Pre-exponential factor of the reverse reaction.
<i>ea_rev</i>	real	Activation energy of the reverse reaction (kJ/mol).
<i>stoic</i>	real	The stoichiometric coefficient.
<i>rate_power</i>	real	The exponent in the rate law.

Table 3. Main input data file (continued)

Input variable	Format	Description
<i>fl_mult</i>	real	Parameter signifying whether this particular reaction occurs for this solute in the fluid phase.
<i>sb_mult</i>	real	Parameter signifying whether this particular reaction occurs for this solute in the sorbed phase.
<i>h_mult</i>		For Henry's Law species, parameter signifying whether this particular reaction occurs for the liquid-borne or vapor-borne portion of the species.
<i>macro</i>	character*4	Keyword " sol " (required).
<i>ntt</i>	integer	Parameter that defines the type of solution required.
<i>intg</i>	integer	Parameter that defines element integration type.
<i>macro</i>	character*4	Keyword " solv " (not implemented).
<i>macro</i>	character*4	Keyword " stea " (optional; no input is associated with this macro).
<i>macro</i>	character*4	Keyword " strs " (not implemented in this version of FEHM).
<i>macro</i>	character*4	Keyword " svar " (optional).
<i>ivar</i>	integer	To enable pressure-enthalpy variables in place of pressure temperature for water/water-vapor physics, <i>ivar</i> = 1.
<i>macro</i>	character*4	Keyword " text " (optional).
<i>wdd1</i>	character*80	Line of text. A maximum of 80 characters per line are entered. A blank line to signal end of text input.
<i>macro</i>	character*4	Keyword " thic " (optional).
<i>ja, jb, jc</i>	integer	See description under keyword " boun " (page 37).
<i>thic</i>	real	Thickness of the model domain in the third dimension (m). A blank line to signal end of thickness input.
<i>macro</i>	character*4	Keyword " time " (required).
<i>day</i>	real	Initial time-step size (days).
<i>tims</i>	real	Final simulation time (days).
<i>nstep</i>	integer	Maximum number of time steps allowed.
<i>ii</i>	integer	Print-out interval for nodal information (pressure, enthalpy, etc.) as set up under control-statement node (i.e., number of time steps).
<i>year</i>	integer	Year that simulation starts.
<i>month</i>	integer	Month that simulation starts.
<i>initime</i>	real	Initial time of simulation.
<i>dit1</i>	real	Time (days) for time-step change.
<i>dit2</i>	real	New time-step size (days).
<i>dit3</i>	real	Implicitness factor for new time step.
<i>itc</i>	integer	New print-out interval. A blank line to signal end of time-step change input.
<i>macro</i>	character*4	Keyword " trac " (optional).
<i>user_macro</i>	character*5	Key word for invoking a solute-transport user subroutine.
<i>ano</i>	real	Initial solute concentration.
<i>awc</i>	real	Implicitness factor for solute solution.
<i>epc</i>	real	Equation tolerance for solute solution.
<i>upwgta</i>	real	Upstream weighting term for the solute solution.

Table 3. Main input data file (continued)

Input variable	Format	Description
<i>daycs</i>	real	Time for which the solute solution is enabled (days).
<i>daycf</i>	real	Time for which the solute solution is disabled (days).
<i>dayhf</i>	real	Time for which the flow solution is disabled (days).
<i>dayhs</i>	real	Time for which the flow solution is enabled (days).
<i>iaccmx</i>	integer	Maximum number of iterations allowed in solute solution if time-step multiplier is enabled.
<i>daycm</i>	real	Time-step multiplier for solute solution.
<i>daycmm</i>	real	Minimum time step for solute solution (days).
<i>daycmx</i>	real	Maximum time step for solute solution (days).
<i>nspecies</i>	integer	Number of solutes simulated.
<i>input_msg</i>	character*4	Keyword ' <i>ldsp</i> ' specifying longitudinal/transverse dispersion is desired.
There are two options for dispersivity and sorption parameters.		
<i>icns</i>	integer	Phase designation for the <i>ith</i> solute.
<i>iadsf</i>	integer	Adsorption model type for the <i>ith</i> species, <i>ith</i> region.
<i>a1adsf</i>	real	α_1 parameter in adsorption model.
<i>a2adsf</i>	real	α_2 parameter in adsorption model.
<i>betadf</i>	real	β parameter in adsorption model.
<i>diffm</i>	real	Molecular diffusion coefficient (m^2/s).
<i>tcx, tcy, tcz</i>	real	Dispersivity in the x-, y-, z-directions (m).
<i>ja, jb, jc</i>	integer	See description under keyword " boun " (page 37).
<i>itrcd</i>	integer	Region number for sorption and dispersion parameters given above.
A blank line to signal end of region input.		
or		
<i>input_msg</i>	character*4	Keyword specifying that the same diffusion coefficient and dispersivities are to be used for all species of the same type (liquid and/or vapor): ' <i>dspl</i> ' - liquid only, ' <i>dspv</i> ' - vapor only, ' <i>dspb</i> ' - both liquid and vapor.
<i>diffm</i>	real	Molecular diffusion coefficient (m^2/s) for liquid or vapor only.
<i>tcx, tcy, tcz</i>	real	Dispersivity in the x-, y-, z-directions (m) for liquid or vapor only.
or		
<i>diffml</i>	real	Molecular diffusion coefficient (m^2/s) for liquid.
<i>tcxl, tcyl, tczl</i>	real	Dispersivity in the x-, y-, z-directions (m) for liquid.
<i>diffmv</i>	real	Molecular diffusion coefficient (m^2/s) for vapor.
<i>tcxv, tcyv, tczv</i>	real	Dispersivity in the x-, y-, z-directions (m) for vapor.
<i>ja, jb, jc</i>	integer	See description under keyword " boun " (page 37).
<i>itrcdsp</i>	integer	Region number for dispersion parameters given above.
A blank line to signal end of region input.		
<i>icns</i>	integer	Phase designation for the <i>ith</i> solute.
<i>iadsf</i>	integer	Adsorption model type for the <i>ith</i> species, <i>ith</i> region.
<i>a1adsf</i>	real	α_1 parameter in adsorption model.
<i>a2adsf</i>	real	α_2 parameter in adsorption model.
<i>betadf</i>	real	β parameter in adsorption model.
<i>ja, jb, jc</i>	integer	See description under keyword " boun " (page 37).
<i>itrcd</i>	integer	Region number for sorption parameters given above.
A blank line to signal end of region input.		
The data that follow apply to either of the sorption/dispersivity input options used above.		

Table 3. Main input data file (continued)

Input variable	Format	Description
<i>henry_model</i>	integer	Flag denoting which model is to be used for defining the temperature dependence of the Henry's Law constant.
<i>hawwa(1)</i>	real	Term in Henry's Law temperature-dependence model: model 1 - $A_{H,1}$, model 2 - $A_{H,1}$
<i>hawwa(2)</i>	real	Term in Henry's Law temperature-dependence model: model 1 - ΔH_H , model 2 - $A_{H,2}$
<i>hawwa(3)</i>	real	Term in Henry's Law temperature-dependence model 2 - $A_{H,3}$.
<i>hawwa(4)</i>	real	Term in Henry's Law temperature-dependence model 2 - $A_{H,4}$.
<i>hawwa(5)</i>	real	Term in Henry's Law temperature-dependence model 2 - $A_{H,5}$.
<i>ja, jb, jc</i>	integer	See description under keyword " boun " (page 37).
<i>anqo</i>	real	Initial concentration of tracer, which will supersede the value given by <i>ano</i> .
A blank line to signal end of concentration input.		
<i>ja, jb, jc</i>	integer	See description under keyword " boun " (page 37).
<i>cnsk</i>	real	Injection concentration at inlet node (moles per kg liquid or vapor).
<i>t1sk</i>	real	Time (days) when tracer injection begins.
<i>t2sk</i>	real	Time (days) when tracer injection ends.
A blank line to signal end of tracer injection input.		
<i>macro</i>	character*4	Keyword " user ".
<i>kk</i>	integer	Integer number passed to subroutine <i>user</i> for user-defined input parameters.
<i>macro</i>	character*4	Keyword " vcon ".
<i>ivcon(i)</i>	integer	Model type for <i>ith</i> conductivity model: linear variation of thermal conductivity with temperature or square-root variation of thermal conductivity with liquid saturation.
<i>vc1f(i)</i>	real	Reference temperature ($^{\circ}\text{C}$) or conductivity ($\frac{W}{m \cdot K}$) at liquid saturation = 1, depending on model.
<i>vc2f(i)</i>	real	Reference conductivity ($\frac{W}{m \cdot K}$) or conductivity ($\frac{W}{m \cdot K}$) at liquid saturation = 0, depending on model.
<i>vc3f(i)</i>	real	Change in conductivity with respect to temperature or not used, depending on model.
A blank line to signal end of conductivity-model input.		
<i>ja, jb, jc</i>	integer	See description under keyword " boun " (page 37).
<i>ivcnd</i>	integer	Number referring to the sequence of models read.
A blank line to signal end of conductivity-model desingator input.		
<i>macro</i>	character*4	Keyword " velo ". The input is identical to " flxo " except that velocities instead of fluxes are calculated (see page 40).
<i>macro</i>	character*4	Keyword " wlbr " (not supported this version).
<i>macro</i>	character*4	Keyword " zone " (optional). See Section 4.1.4.2.4 on page 49.
<i>macro</i>	character*4	Keyword " stop ".

4.1.4.2.3 Geometry data file. The geometry data file contains the mesh element and coordinate data (Table 4). This information can either be part of the main input file or a separate file.

Table 4. Geometry data file		
Input variable	Format	Description
<i>macro</i>	character*4	Keyword " coor ".
<i>n</i>	integer	Number of nodes in the grid.
For each node:		
<i>mb</i>	integer	Node number. If $mb < 0$, then the difference between the absolute value of mb and the previously read absolute value of mb is used to generate intermediate values by interpolation.
<i>cord(mb,1)</i>	real	X-coordinate of node mb (m).
<i>cord(mb,2)</i>	real	Y-coordinate of node mb (m).
<i>cord(mb,3)</i>	real	Z-coordinate of node mb (m).
A blank line to signal end of node input.		
<i>macro</i>	character*4	Keyword " elem ".
<i>ns</i>	integer	Number of nodes per element.
<i>nei</i>	integer	Number of elements.
For each element:		
<i>mb</i>	integer	Element number. If $mb < 0$, then the difference between the absolute value of mb and the previous absolute value of mb is used to generate intermediate values by interpolation in the code.
<i>nelm(k)</i>	integer	ns node numbers for the nodes in element mb ($k = (mb - 1) * ns + i$, $i = 1$ to ns).
A blank line to signal end of element input.		
<i>macro</i>	character*4	Keyword " stop ".

4.1.4.2.4 Zone data file. The zone data file contains the zone information, which can either be part of the main input file or a separate file (Table 5).

Table 5. Zone data file		
Input variable	Format	Description
<i>macro</i>	character*4	Keyword " zone ".
For each geometric zone:		
<i>izone</i>	integer	Zone identification number.
Followed by:		
<i>xz(i)</i>	real	X-coordinates defining zone <i>izone</i> .
<i>yz(i)</i>	real	Y-coordinates defining zone <i>izone</i> .
<i>zz(i)</i>	real	Z-coordinates defining zone <i>izone</i> .
Note: $i = 1$ to 4 for 2-D and zz is not input, $i = 1$ to 8 for 3-D.		
or		
<i>macro</i>	character*4	Keyword " list ".
<i>xg</i>	real	A list of x-, y-, z-coordinates, one set per line until a blank line is encountered (zg is not input for 2D). The nodes corresponding to these coordinates make up <i>izone</i> .
<i>yg</i>	real	
<i>zg</i>	real	

Table 5. Zone data file (continued)

Input variable	Format	Description
or		
<i>macro</i>	character*4	Keyword "nnum".
<i>nin</i>	integer	Specified number of nodes.
<i>node(i)</i>	integer	<i>nin</i> node numbers of the nodes to be included in <i>izone</i> (<i>i</i> = 1 to <i>nin</i>).
A blank line to signal end of zone input.		
<i>macro</i>	character*4	Keyword "stop".

4.1.4.2.5 Optional input files. The optional input files contain data for specified macros using the macro formats described above in Section 4.1.4.2.2 and Section 4.1.4.2.4 of this chapter.

4.1.4.2.6 Restart input file. The restart input data file provides **fehm** initial values of pressure, temperature, saturation, and simulation or starting time. See Section 4.1.4.4.2 (Table 7) for variable names, format, and description. The code version, date, time, and problem title contained in the file are not used for input, but that information or two blank lines must be present for the file to be read correctly.

4.1.4.2.7 Coefficient storage file. The coefficient storage input file contains finite-element coefficients calculated by the code during a previous run. See Section 4.1.4.4.7 (Table 9) of this chapter for variable names, format, and description. The code version, date, time, and problem title contained in the file are not used for input, but that information or two blank lines must be present for the file to be read correctly.

4.1.4.3 Prompted input

Input prompts are used only when the default control file (*fehmn.files*) is not present in the directory from which the code is being executed. Table 6 below lists the prompts and expected responses. If the initial prompt is answered with the name of an input control file (see Section 4.1.4.2.1 in this chapter above), no further prompts will be issued and the remainder of the I/O data will be read from the control file. If the I/O data is not accepted (final prompt answered "no"), the prompts will be repeated starting with request for the control file name. The terminal display that accompanies input prompting is shown in Section 4.1.4.5.1 of this chapter.

A carriage return, <cr>, refers to a return with no input that accepts the displayed default value. Responses to file name queries may be the name of a file (including path or subdirectories), <cr>, or either "na" or "not using" to indicate the file is not required by the user. Prompts that use the input file name response are denoted <input> or <root> (input file name without suffix).

Table 6. Prompted input

Input prompt	Format	Expected response
Enter name for iocntl -- default file name: not using [(name/na or not using), RETURN = DEFAULT]	character*100	Input control file name, <cr>, or either "na" or "not using".
Enter name for inpt -- default file name: fehmn.dat [(name/na or not using), RETURN = DEFAULT]	character*100	Input file name or <cr> to use the default name.
Do you want all file names of the form <root of input file name>.* ? [(y/n), RETURN = y] *** Note: If "y" incoor and inzone will equal inpt *** Note: The next 11 filename prompts are issued only if the previous prompt was answered with "n".	character*100	"y" or "n".
Enter name for incoor -- default file name: <input> [(name/na or not using), RETURN = DEFAULT]	character*100	Geometry data file name, <cr>, or either "na" or "not using".
Enter name for inzone -- default file name: <input> [(name/na or not using), RETURN = DEFAULT]	character*100	Zone data file name, <cr>, or either "na" or "not using".
Enter name for iout -- default file name: <root>.out [(name/na or not using), RETURN = DEFAULT]	character*100	Output file name or <cr> to use the default name.
Enter name for iread -- default file name: <root>.ini [(name/na or not using), RETURN = DEFAULT]	character*100	Restart input file name, <cr>, or either "na" or "not using".
Enter name for isave -- default file name: <root>.fin [(name/na or not using), RETURN = DEFAULT]	character*100	Restart output file name, <cr>, or either "na" or "not using".
Enter name for ishis -- default file name: <root>.his [(name/na or not using), RETURN = DEFAULT]	character*100	History plot file name, <cr>, or either "na" or "not using".
Enter name for istrc -- default file name: <root>.trc [(name/na or not using), RETURN = DEFAULT]	character*100	Solute plot file name, <cr>, or either "na" or "not using".
Enter name for iscon -- default file name: <root>.con [(name/na or not using), RETURN = DEFAULT]	character*100	Contour plot file name, <cr>, or either "na" or "not using".
Enter name for iscon1 -- default file name: <root>.dp [(name/na or not using), RETURN = DEFAULT]	character*100	Contour plot file name for dual or dpdp, <cr>, or either "na" or "not using".
Enter name for isstor -- default file name: <root>.stor [(name/na or not using), RETURN = DEFAULT]	character*100	Coefficient storage file name, <cr>, or either "na" or "not using".
Enter name for ischk -- default file name: <root>.chk [(name/na or not using), RETURN = DEFAULT]	character*100	Input check output file name, <cr>, or either "na" or "not using".
tty output -- show all reference nodes, selected reference nodes, or none: [(all/some/none), RETURN = none]	character*4	"all", "some", or "none".

Table 6. Prompted input (continued)

Input prompt	Format	Expected response
user subroutine number (provided to subroutine USER before every time step): [RETURN = none]	integer	Number of user subroutine, <cr>, or "0" for not using.
If data is OK enter yes to continue, no to restart terminal input, or stop to end program: [(yes/no/stop), RETURN = yes]	character*4	"yes", "no", or "stop".

4.1.4.4 Output files

4.1.4.4.1 Main output file. The main output file records the code version, date, and time followed by the user-input problem title. A summary of the I/O files used, macro control statements read, and array storage follow. Timing, equation performance, nodal (for user-specified nodes), and global mass- and energy-balance information at user-selected time intervals is written in a narrative format. See Section 4.1.4.5.2 in this chapter for an example of the information output and narrative style. The file ends with a summary of simulation time, number of time steps in the problem, the number of iterations taken, and total cpu time. The default output file name is *fehmn.out*.

4.1.4.4.2 Restart output file. The restart output data file stores **fehmn** final values of pressure, temperature, saturation, and simulation time (Table 7). The default restart output file name is *fehmn.fin*.

Table 7. Restart output file

Output variable	Format	Description
verno	character*20	Code version
jdate	character*11	Date
jtime	character*8	Time
wdd	character*80	Problem title
days	real*8	Simulation time (days)
wdd1(1:4)	character*4	Gas problem flag (ngas, h20, air)
wdd1(5:8)	character*4	Tracer problem flag (trac, ntra)
wdd1(9:12)	character*4	Stress problem flag (strs, nstr)
wdd1(13:16)	character*4	Double-porosity/double-permeability problem flag (dpdp, ndpd)
wdd1(17:20)	character*4	Dual-porosity problem flag (dual, ndua)
t(ncount)	real*8	Temperature (not present when air flag is set, isothermal air/water problem)
s(ncount)	real*8	Liquid saturation
phi(ncount)	real*8	Pressure
pci(ncount)	real*8	Gas pressure (only present if noncondensable gas problem, ngas flag is set).
Array dimension ncount = neq, the number of nodes in the problem; if dpdp flag is set, ncount = 2*neq; if dual flag is set, ncount = 3*neq		

4.1.4.4.3 Simulation history output file. The history plot file records parameter values at selected nodes for each time step of the simulation (Table 8). The default history output file name is *fehmh.his*.

Table 8. Simulation history output file		
Output variable	Format	Description
verno	character*20	Code version
jdate	character*11	Date
jtime	character*8	Time
wdd	character*80	Problem title
N/A	character*4	Tracer problem flag ('trac' or blank)
N/A	character*4	Stress problem flag ('strs' or blank)
m	integer	Number of nodes for which data are output
mi	integer	Node number
cord(mi,*)	real*8	X-, y-, and z-coordinate of each node for which data are output (m sets)
N/A	character	Data headings (3 lines) as follows: headings node flow enthalpy(Mj/kg) flow(kg/s) temperature(deg C) total pressure (Mpa) capillary pressure(Mpa) saturation(kg/kg)
For each time step:		
days	real*8	Simulation time
followed by (for each specified output node):		
mi	integer	Node number
qh(mi)	real*8	Energy source (MJ/s)
sk(mi)	real*8	Source strength (kg/s)
t(mi)	real*8	Temperature (°C)
phi(mi)	real*8	Pressure (MPa)
pcp(mi)	real*8	Capillary pressure (MPa)
s(mi)	real*8	Saturation (dimensionless)

4.1.4.4.4 Solute history output file. The solute history plot file records solute parameter values at selected nodes for each time step of the simulation (Table 9). The default solute history output file name is *fehmh.trc*.

Table 9. Solute history output file		
Output variable	Format	Description
verno	character*20	Code version
jdate	character*11	Date
jtime	character*8	Time
wdd	character*80	Problem title
m	integer	Number of nodes for which data are output
mi	integer	Node number
cord(mi,*)	real*8	X-, y-, and z-coordinate of each node for which data are output (m sets)
nspeci	integer	Number of different species for tracer solution

Table 9. Solute history output file (continued)

Output variable	Format	Description
For each time step:		
days	real*8	Simulation time
nsp	integer	Species number
followed by (for each specified output node):		
an(mi)	real*8	Species concentration (dimensionless)

4.1.4.4.5 Contour plot output file. The contour plot records parameter values for each node at selected time steps of the simulation (Table 10). The default contour plot output file name is *fehmn.con*.

Table 10. Contour plot output file

Output variable	Format	Description
verno	character*20	Code version
jdate	character*11	Date
jtime	character*8	Time
wdd	character*80	Problem title
N/A	character*4	Tracer problem flag ('trac' or blank)
N/A	character*4	Stress problem flag ('strs' or blank)
neq	integer	Number of nodes for which data are output
cord(i,*)	real*8	X-, y-, and z-coordinate of each node for which data is output (neq sets)
ns	integer	Number of nodes per element, total number of elements
nei	integer	
nelm(ns)	integer	Nodal connectivity information for each node of each element
pnx(neq)	real*8	X-, y-, z-permeability (m ²) for each node
pny(neq)	real*8	
pnz(neq)	real*8	
thx(neq)	real*8	X-, y-, z-thermal conductivity ($\frac{W}{m \cdot K}$) for each node
thy(neq)	real*8	
thz(neq)	real*8	
ps(neq)	real*8	Porosity, rock specific heat ($\frac{MJ}{kg \cdot K}$), capillary pressure (MPa) for each node
cpr(neq)	real*8	
pcp(neq)	real*8	
idof	integer	Number of degrees of freedom per node for the current problem
igrav	integer	Direction of gravity in problem
grav	real*8	Value of gravity
nspeci	integer	Number of species if tracer solution is present
For each specified time step:		
days	real*8	Simulation time
inj	real*8	Injection phase (≥ 0 : liquid; < 0 : vapor)

Table 10. Contour plot output file (continued)

Output variable	Format	Description
If injection phase is liquid, for each node:		
N/A	real*8	Liquid transmissibility/density [dil(neq)/rolf(neq)]
rolf(neq)	real*8	Liquid density
N/A	real*8	Pressure - capillary pressure [phi(neq) - pcp(neq)]
t(neq)	real*8	Temperature
If injection phase is vapor, for each node:		
N/A	real*8	Vapor transmissibility/density [div(neq)/rovf(neq)]
rovf(neq)	real*8	Vapor density
phi(neq)	real*8	Pressure
t(neq)	real*8	Temperature
If tracer solution is present, for each species, for each node:		
an(neq) or	real*8	Species concentration of liquid phase or vapor phase
anv(neq)	real*8	

4.1.4.4.6 Dual-porosity or double-porosity/double-permeability contour plot output file. The dual-porosity or double-porosity/double-permeability contour plot file records parameter values for each dpdp (neq + 1 to 2*neq) or dual (neq + 1 to 3*neq) node at selected time steps of the simulation (Table 11). This file contains the same information as the regular contour plot file (see Table 10 above). The default dual-porosity or double-porosity/double-permeability contour plot output file name is *fehmn.dp*.

4.1.4.4.7 Coefficient storage file. The coefficient storage output file contains finite-element coefficients calculated by the code. The default coefficient storage file name is *fehmn.stor*.

Table 11. Coefficient storage file

Output variable	Format	Description
verno	character*20	Code version
jdate	character*11	Date
jtime	character*8	Time
wdd	character*80	Problem title
iwtotl	integer	Number of storage locations needed to store geometric input types
neq	integer	Number of nodes
ncont	integer	Number of positions for which information needs to be stored
sx1(neq)	real*8	Volume associated with each node
nelm(ncont)	integer	Nodal-connectivity information for each connection
istrw(ncont)	integer	Starting position for each connection
nelmdg(neq)	integer	Position of element in connectivity array for each node
sx(iwtotl)	real*8	Finite-element geometric coefficient for each storage location
sxs(iwtotl)	real*8	Finite-element geometric coefficient for each storage location for stress module if enabled

4.1.4.4.8 Input check output file. The input check output file contains a summary of input information that may be of use in debugging or memory management of the code. The positions of maximum and minimum values of input parameters and derived quantities are given. Also provided is an analysis of array storage requirements. The default input check output file name is *fehmn.chk*.

4.1.4.4.9 Error output file. The error output file contains any error or warning messages issued by the code during a run (Table 12). The default error output file name is *fehmn.err*.

Table 12. Error output file		
Output variable	Format	Description
verno	character*20	Code version
jdate	character*11	Date
jtime	character*8	Time
wdd	character*80	Problem title
N/A	character	Warning and/or error messages issued during code execution (see Section 4.1.4.6 for a summary of possible messages)

4.1.4.4.10 AVS log output file. The AVS log output file provides a record of AVS data output files names and corresponding simulation time (Table 13).

Table 13. AVS log output file		
Output variable	Format	Description
	character*2	"# "
verno	character*20	Code version
jdate	character*11	Date
jtime	character*8	Time
N/A	character*80	Heading : # LOG AVS OUTPUT
	character*2	"# "
wdd	character*80	Problem title
Blank line followed by (for each AVS data file written):		
root	character*95	Filename root
icall	integer	File number (appended to root)
days	real*8	Simulation time (days)

4.1.4.4.11 AVS header output files. The AVS ASCII header file contains information about the AVS output files and one line of header data as follows (Table 14).

Table 14. AVS ASCII header output files		
Output variable	Format	Description
	character*2	"# "
verno	character*20	Code version
jdate	character*11	Date

Table 14. AVS ASCII header output files (continued)		
Output variable	Format	Description
N/A	character*80	Heading : # AVS UNSTRUCTURED CELL DATA (UCD) FROM FEHM
	character*2	"# "
wdd	character*80	Problem title
N/A	character	Text as follows: # ***** # To prepare files for input to avs one must # concatenate header/geometry/node_value files. # For example, if your FEHM input file was fe.dat, # headers are fe10001_sca_head fe10001_vec_head, ..., # mesh geometry will be in fe10001_geo, # field output will be in fe10001_sca_node, # fe10001_vec_node, fe10001_con_dual_node # # A UCD input file can be produced using # cat fe10001_sca_head fe10001_geo fe10001_sca_node > # fe10001_sca_node.inp # # The UNIX for each command is useful for processing # multiple files. Also use the shell script fehm2avs # to perform automatic processing of all output. # *****
neq	integer	Number of nodes
nei	integer	Number of cells (elements)
num_ndata	integer	Number of data components for the nodes
num_cdata	integer	Number of data components for the cells (0)
num_mdatar	integer	Number of data components for the model (0)

The AVS binary header file contains only the header data as follows in 21 bytes (Table 15).

Table 15. AVS binary header output files		
Output variable	Format	Description
	1 byte int	The number "7" indicating binary file
num_nodes	4 byte int	Number of nodes
num_cells	4 byte int	Number of cells (elements)
num_node_data	4 byte int	Number of data components for the nodes
num_cell_data	4 byte int	Number of data components for the cells (0)
num_model_data	4 byte int	Number of data components for the model (0)

4.1.4.4.12 AVS geometry output file. The AVS geometry file contains node, coordinate, cell, and material data. The ASCII file contains the data as follows (Table 16).

Table 16. AVS ASCII geometry output file		
Output variable	Format	Description
i	integer	Node id
x, y, z	real*8	X-, y-, z-coordinate for each node
i	integer	Cell id
ipropelm	integer	Material id
char_type	character*5	Cell type
nelm	integer	List of cell vertices for each cell

The binary (unformatted) file contains the data as follows (Table 17).

Table 17. AVS binary geometry output file		
Output variable	Format	Description
num_nlist	4 byte int	Number of nodes in connection list
i	4 byte int	Cell id
ipropm	4 byte int	Material id
ns	4 byte int	Num nodes
elem_type	4 byte int	Cell type - cell information for each cell
np	num_nlist 4 byte ints	Node list - cell topology (connectivity list)
x	num_nodes 4 byte floats	X-coordinates
y	num_nodes 4 byte floats	Y-coordinates
z	num_nodes 4 byte floats	Z-coordinates

4.1.4.4.13 AVS data output files. The ASCII node data files contain the number of data components and size, a label/unit description for each data component, and the associated data for each node as follows (Table 18).

Table 18. AVS ASCII data output files		
Output variable	Format	Description
N/A	integer	Number of data components and size
title	character*80	Variable label and output units for each data component
Material properties data output for each node.		
i	integer	Node
pnx, pny, pnz	real*8	Permeability in x-, y-, and z-direction (m^2)
thx, thy, thz	real*8	Thermal conductivity in x-, y-, and z-direction ($\frac{W}{m \cdot K}$)
ps	real*8	Porosity
cpr	real*8	Rock specific heat ($\frac{MJ}{kg \cdot K}$)
pcp	real*8	Capillary pressure (MPa)
irlp	real*8	Relative-permeability model
icap	real*8	Capillary-pressure model

Table 18. AVS ASCII data output files (continued)

Output variable	Format	Description
Scalar parameters that may be output for each node (up to 4).		
i	integer	Node
s	real	Saturation
t	real	Temperature (°C)
phi	real	Liquid pressure (MPa)
phi - pcp	real	Vapor pressure (MPa)
Vector parameters that may be output for each node.		
pnxl, pnyl, pnzl	real	Liquid velocity (m/s), x-, y-, and z-component
pnxv, pnyv, pnzv	real	Vapor velocity (m/s), x-, y-, and z-component
Solute concentrations that may be output for each node (up to 20).		
an	real	Tracer concentration

The binary (unformatted) AVS data files use the following format for the data types described above (Table 19).

Table 19. AVS binary data output files

Output variable	Format	Description
See previous table	1024 byte string	Node data labels
	1024 byte string	Node data units
	4 byte int	Number of node components
	4 byte floats	Node-component list
	4 byte floats	Minimums for node data
	4 byte floats	Maximums for node data
	4 byte floats	Data blocks with values for each node

4.1.4.5 Displays and reports

4.1.4.5.1 I/O prompt display. The following file description display appears on the screen when **feh** is executed and I/O prompts are invoked (see Section 4.1.4.3 in this chapter above).

version FEHM 01.00 [*machine*] 96/05/29 15:34:29

**** Default names for I/O files ****

```

control file      : fehmn.files
input file       : filen.*
geometry data file: filen.*
zone data file   : filen.*
output file      : filen.out
read file (if it exists): filen.ini
write file (if it exists): filen.fin
history plot file: filen.his
tracer history plot file: filen.trc

```

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contour plot file: filen.con
dual or dpdp contour plot file: filen.dp
stiffness matrix data read/write file: filen.stor
input check file : filen.chk

**** where ****

"filen.*" may be 100 characters maximum. If a name is not entered when prompted for, a default file name is used. "fehmน์.dat" is the default used for the input file name.

**** note ****

A save file and input check file are always written. If you do not provide a name for these files, the following defaults will be used: fehmน์.fin, fehmน์.chk.

After terminal I/O has been completed, the following display reporting what was input (user-input responses shown in < >) is shown prior to the prompt asking if the I/O data are OK.

Not using tty output <none> or First reference output node will be written to tty <some> or All reference output nodes will be written to tty <all>

File purpose - Variable - Unit number - File name

control	- iocntl	- 0	- not using
input	- inpt	- 11	- <input file name>
geometry	- incoor	- 11	- <geometry data file name>
zone	- inzone	- 11	- <zone data file name>
output	- iout	- 14	- <output data file name>
initial state	- iread	- 0	- <restart input file name>
final state	- isave	- 16	- <restart output file name>
time history	- ishis	- 17	- <history plot file name>
time his.(tr)	- istr	- 18	- <solute history plot file name>
contour plot	- iscon	- 19	- <contour plot file name>
con plot (dp)	- iscon1	- 20	- <dp contour plot file name>

fe coef stor - isstor- 21 - <coefficient storage file name>

input check - ischk- 22 - <input check output file name>

Value provided to subroutine user: <user subroutine number>

4.1.4.5.2 Terminal run time display. If terminal output is invoked (tty_flag "all" or "some"), a summary of the I/O files used (as shown above in Section 4.1.4.5.1 of this chapter) is displayed. This information is followed by the maximum number of nodes in the problem, the problem title, macro control statements read, and array storage parameters as shown in the example on the next page. The output marked with a "bar" is displayed only when the "all" flag is used.

n0 = 9

***** 2-D Heat Conduction Model *****

```

**** input title : coor **** incoor = 12 ****
**** input title : elem **** incoor = 12 ****
**** input title : stop **** incoor = 12 ****
**** input title : zone **** inzone = 13 ****
**** input title : stop **** inzone = 13 ****
**** input title : node **** inpt = 11 ****
**** input title : sol **** inpt = 11 ****
**** input title : init **** inpt = 11 ****
**** input title : zone **** inpt = 11 ****
**** input title : rock **** inpt = 11 ****
**** input title : cond **** inpt = 11 ****
**** input title : perm **** inpt = 11 ****
**** input title : flow **** inpt = 11 ****
**** input title : time **** inpt = 11 ****
**** input title : ctrl **** inpt = 11 ****
**** input title : stop **** inpt = 11 ****

```

pressures and temperatures set by gradients

storage needed for ncon43 available43
storage needed for nop43 available46
storage needed for a matrix33 available33
storage needed for b matrix33 available46
storage needed for gmres81 available81
storage available for b matrix resized to

33<<<<<<

time for reading input, forming coefficients 0.667E-01

**** analysis of input data on file fehmn.chk

volumes and fe coefficients checked

storage for fe coefficients 12 allocated 12

Information that is displayed at each time step if either tty_flag is used is illustrated below. This information includes timing, equation performance, and mass and energy balances. The output marked with a "bar" is displayed at selected time steps for the selected output nodes only when the "all" flag is used. Additional parameters may be displayed depending on the type of problem (i.e., transport or double porosity) being executed.

Time Step 1

Timing Information

Years	Days	Step Size (Days)
0.136893E-04	0.500000E-02	0.500000E-02

Cpu Sec for Time Step = 0.3932E-02 Current Total = 0.1184E-01

Equation Performance

Number of N-R Iterations: 1
Avg # of Linear Equation Solver Iterations: 3.0
Number of Active Nodes: 9.
Total Number of Newton-Raphson Iterations: 1

Largest Residuals

EQ1 R= 0.1660E-07 node= 5 x=0.2500 y=0.2500 z= 1.000

Node	Equation 1 Residual	Equation 2 Residual
5	0.165983E-07	0.135450E+01
7	0.111444E-07	0.185894E-01

Nodal Information (Water)

Node	p(MPa)	e(MJ)	I sat	temp(c)	source/sink	
					(kg/s)	(MJ/s)
5	10.000	0.00	0.000	198.645	0.	0.
7	10.000	0.00	0.000	199.981	0.	0.

Time Step 2

Timing Information		
Years	Days	Step Size (Days)
0.273785E-04	0.100000E-01	0.500000E-02
Cpu Sec for Time Step = 0.3274E-02 Current Total = 0.2175E-01		
Equation Performance		
Number of N-R Iterations: 1		
Avg # of Linear Equation Solver Iterations: 3.0		
Number of Active Nodes: 9.		
Total Number of Newton-Raphson Iterations: 2		
Largest Residuals		
EQ1 R= 0.3765E-08 node= 5 x=0.2500 y=0.2500 z= 1.000		
Global Mass & Energy Balances		
Total mass in system at this time: 0.000000E+00 kg		
Total mass of steam in system at this time: 0.000000E+00 kg		
Total enthalpy in system at this time: 0.104781E+03 MJ		
Water discharge this time step: 0.000000E+00 kg		
Water input this time step: 0.000000E+00 kg		
Total water discharge: 0.000000E+00 kg		
Total water input: 0.000000E+00 kg		
Enthalpy discharge this time step: 0.342068E+00 MJ		
Enthalpy input this time step: 0.000000E+00 MJ		
Total enthalpy discharge: 0.301221E+02 MJ		
Total enthalpy input: 0.301221E+02 MJ		
Net kg water discharge (total out-total in): 0.000000E+00		
Net MJ discharge (total out-total in): 0.000000E+00		
Conservation Errors: 0.000000E+00 (mass), -0.100323E+01 (energy)		
Time Step	3	
.		
.		
.		

4.1.4.6 Messages

Fatal error conditions and messages for the **feh**m program are given in Table 20. Warning messages (nonfatal errors or informational messages) are given in Table 21.

Table 20. Error conditions that result in program termination	
Error condition	Error message
I/O file error	
Unable to open I/O file	<p>**** Error opening file <i>fileid</i> ****</p> <p>◇</p> <p>◇</p> <p>◇</p> <p>****-----****</p> <p>**** JOB STOPPED ****</p> <p>****-----****</p>
Coefficient storage file not found	program terminated because coefficient storage file not found
Optional rlp file not found	relative perm file does not exist: stopping
Optional input file not found	ERROR nonexistent file <i>filename</i>
Unable to open optional input file	STOPPED trying to use optional input file
Unable to determine file prefix for AVS output files	ERROR opening <i>filename</i>
	STOPPED trying to use optional input file
	FILE ERROR: nmfil2 file: <i>filename</i> unable to determine contour file prefix
Input deck errors	
Coordinate or element data not found	<p>**** COOR Required Input ****</p> <p>-or-</p> <p>**** ELEM Required Input ****</p> <p>****-----****</p> <p>**** JOB STOPPED ****</p> <p>****-----****</p>
Invalid macro read	**** error in input deck : <i>char</i> ****
Invalid AVS keyword read for macro cont	<p>ERROR:READ_AVS_IO</p> <p>unexpected/invalid character string <i>string</i></p> <p>.</p> <p>.</p> <p>.</p>
Invalid parameter values (macros using loop construct)	<p>Terminate program execution</p> <p>Fatal error - for array number <i>arraynum</i></p> <p>macro - <i>macro</i> Group number - <i>groupnum</i></p> <p>Something other than a real or integer has been specified</p> <p>-or-</p> <p>Line number - <i>line</i></p> <p>Bad input, check this line</p>
Invalid tracer input	<p>** Using Old Input Enter Temperature Dependency</p> <p>Model Number: 1 - Van Hoff 2 - awwa model, see manual for details **</p>

Table 20. Error conditions that result in program termination (continued)	
Error condition	Error message
Invalid transport conditions	Fatal error. You specified a Henrys Law species with initial concentrations input for the vapor phase (icns = -2), yet the Henrys Constant is computed as 0 for species number <i>speciesnum</i> and node number <i>nodenum</i> . If you want to simulate a vapor-borne species with no interphase transport, then you must specify a gaseous species (icns = -1).
Invalid flag specified for diffusion coefficient calculation	ERROR -- Illegal Flag to concadiff Code Aborted in concadiff
Optional input file contains data for wrong macro	ERROR --> Macro name in file for macro <i>macroname</i> is <i>wrong_macroname</i> STOPPED trying to use optional input file
Invalid parameters set	
Dual porosity	**** check fracture volumes, stopping **** **** check equivalent continuum VGs ****
Noncondensable gas	cannot input ngas temp in single phase -or- ngas pressure lt 0 at temp and total press given max allowable temperature <i>temp</i> -or- ngas pressure gt total pressure <i>i</i> = <i>i</i> -or- ngas pressure lt 0.
Particle tracking	ERROR: Pcnsk in ptrk must be either always positive or always negative. Code aborted in set_ptrk.f
Tracer	ERROR: Can not have both particle tracking (ptrk) and tracer input (trac). Code Aborted in concen.f
Insufficient storage	
Geometric coefficients	program terminated because of insufficient storage
Dual porosity	***** n > n0, stopping *****
Too many negative volumes or finite-element coefficients	too many negative volumes: stopping -or- too many negative coefficients : stopping
Unable to compute local coordinates	iteration in zone did not converge, izon = <i>zone</i> please check icnl in macro CTRL
Singular matrix in LU decomposition	singular matrix in ludcmp
Solution failed to converge	timestep less than daymin <i>timestep_number</i> <i>current_timestep_size</i> <i>current_simulation_time</i> -or- Tracer Time Step Smaller Than Minimum Step Stop in resetttrc

Table 21. Warning conditions and messages	
Warning condition	Message
Thermodynamic variables out of bounds (Note: The code will cut the time step until it can successfully finish a time step. Halving of the time step could eventually result in code termination if the solution fails to converge.)	out of bounds:node <i>node_number</i> p= <i>current_fluid_pressure</i> t= <i>current_temperature</i> -or- p= <i>current_fluid_pressure</i> s= <i>current_saturation</i>
Improper parameter set for reacting species	Warning rate_power is not zero for solid species -or- You must specify either 1 or -1 for h_mult. Check your input. Default is to let the liquid in Henrys law react -or- ERROR: FEHM cannot simulate a solid-liquid-vapor rxn -or- No species have been specified for rxn number <i>irxn</i>
Negative volume or finite-element coefficient	warning : negative volume at node <i>i</i> volume = <i>sx1(i)</i> maximum volume = <i>vol_max</i> -or- warning : negative fe coefficient at node <i>i</i> neighbor node <i>ncon(j)</i> coeff sum = <i>sumsx</i> maximum area divided by length = <i>vol_max</i>
Error writing AVS output	
Error opening file	OPEN ERROR: <i>filename</i>
Binary geometry file	WRITE ERROR: geo <i>geometry_file</i> CLOSE ERROR: geo <i>geometry_file</i>
Binary header file	WRITE ERROR: binary header <i>header_file_type</i> CLOSE ERROR: binary header <i>header_file_type</i>
Binary node file	WRITE ERROR: binary node <i>node_file_type</i> CLOSE ERROR: binary node <i>node_file_type</i>
ASCII geometry file (wrong format specified)	AVS_WRITE_CORD Unformatted IO not implemented No action AVS_WRITE_STRUC Unformatted IO not implemented No action
ASCII geometry file (invalid output format)	AVS_WRITE_CORD Invalid output format No action AVS_WRITE_STRUC Invalid output format No action
ASCII scalar node file	----- ERROR: WRITE_AVS_NODE_S nscalar = <i>scalars_requested</i> is greater than maxscalar = <i>max_number_of_scalars</i> Subroutine only able to handle up to 8 scalars -----

Table 21. Warning conditions and messages (continued)

Warning condition	Message
ASCII scalar node file (continued)	----- WARNING: WRITE_AVS_NODE_S Pressure defined, but not Vapor or Liquid There will be no AVS output for scalar pressure -----
	----- WARNING: WRITE_AVS_NODE_S Vapor defined, but not pressure There will be no AVS output for scalar pressure -----
	----- WARNING: WRITE_AVS_NODE_S Liquid defined, but not pressure There will be no AVS output for scalar pressure -----
	----- ERROR: WRITE ASCII NODE S: Unknown IO combination for <i>number</i> scalars pressure, temperature, vapor, saturation, and liquid -----
BINARY scalar node file	----- ERROR: WRITE_BINARY_NODE_V <i>nvector</i> = <i>nvec</i> is greater than <i>maxvector</i> = <i>MAXVECTOR</i> -----
	----- ERROR: WRITE_BINARY_NODE_V Unknown vector value <i>nvec</i> Number beyond bounds: min to max Occurred using <i>pn* i</i> for vector 1 -> <i>pn*</i> <i>*</i> is xl, xv, yl, yv, zl, or zv Number beyond bounds: min to max Occurred using <i>* i</i> for material <i>n</i> -> <i>th*</i> <i>*</i> is pnx, pny, pnz, thx, thy, or thz -----
	ERROR: WRITE_BINARY_NODE_S <i>nscalar</i> = <i>nscalar</i> <i>nmaxscalar</i> = <i>MAXSCALAR</i> -----
	----- WARNING: WRITE_BINARY_NODE_S Pressure defined, but not Vapor or Liquid There will be no AVS output for scalar pressure -----
	----- WARNING: WRITE_BINARY_NODE_S Vapor defined, but not pressure There will be no AVS output for scalar pressure -----
	----- WARNING: WRITE_BINARY_NODE_S Liquid defined, but not pressure There will be no AVS output for scalar pressure -----

Table 21. Warning conditions and messages (continued)	
Warning condition	Message
BINARY scalar node file (continued)	<p>ERROR: WRITE_BINARY_NODE_S: Unknown IO combination for <i>number</i> scalars pressure, temperature, vapor, saturation, and liquid</p> <p>ERROR: WRITE_BINARY_NODE_S Unknown scalar value <i>nscalar</i> Number beyond bounds: min to max Occurred using * i for ? -> pn* * scalar parameter, ? description</p> <p>ERROR: WRITE_BINARY_NODE_CON nspeci = <i>nspeci</i> is greater than max con =</p>

4.1.4.7 Other input/output

N/A

Chapter III:

Verification and Validation Plan

1.0 PURPOSE

The goal of the Verification and Validation (V&V) effort is to test the options and features of the FEHM application that satisfy the requirements specified in Chapter I, "Software Requirements Specification." The current chapter, "Verification and Validation Plan," details the test cases to be performed, many of which were developed for prior versions of FEHM (Zyvoloski et al. 1992; Zyvoloski and Dash 1991a and 1991b), and lists the acceptance criteria that must be satisfied.

2.0 FUNCTIONAL DESCRIPTION

The goal of the verification part of the V&V effort is to check the operation of the code for a variety of simulations. These simulations will encompass the options and features of FEHM that will be used in actual simulations of flow and transport in the unsaturated zone and in modeling and interpreting pressure transient tests, temperature logs, and tracer tests (both conservative and reactive tracers) performed in the saturated zone. The overall verification of FEHM will be accomplished by comparison of results with published analytical solutions and with results from other codes. Because of the nonlinear nature of the water and steam properties, additional verification of the thermodynamics package is included. The verification test cases in Section 4.0 of this chapter are organized in groups based on the functions and features being tested and include: testing of the thermodynamic functions (Section 4.1); heat transfer tests (Sections 4.2 and 4.3); isothermal fluid flow tests (Sections 4.4–4.7); combined heat and mass transfer tests (Sections 4.8–4.11); and solute transport tests (Sections 4.12–4.17).

The model validation part of the V&V effort is in an early stage of development. The goals of validation include modeling of appropriate field tests when experimental data are available from the Yucca Mountain Site Characterization Project. Model validation will not explicitly be discussed in this document but will be included in a later revision when data become available.

3.0 ASSUMPTIONS AND LIMITATIONS

The verification effort assumes that the FEHM application is installed on systems running the UNIX operating system (i.e., Sun Workstations, HP, Cray, IBM, SGI) and that dynamic memory allocation is supported.

When comparing against an analytical solution or other code, it is assumed that close agreement between FEHM and the analytical solution or alternate-model results constitutes a verification of both. Fortuitous agreement between models using entirely different mathematical solution procedures is judged to be extremely unlikely.

The acceptance criteria are based on maximum error, percent error, or root-mean-square (RMS) error. These are standard error measures used in mathematics and the physical sciences. The RMS error indicates average error over the solution domain, and the maximum and percent errors represent the largest errors in the domain. The maximum error is defined to be the absolute value of the maximum difference (error) between the values of the FEHM solution (FS) and the analytical or alternate-model solution (AS), where the error between each point is computed as $Error = abs(AS - FS)$. The percent error (PE) is defined as the error divided by the analytical or alternate-model solution times 100 and is computed for

each point using $PE = abs\left(\frac{AS - FS}{AS}\right) \times 100$. The *RMS* error is calculated using the

following:
$$RMS = \sqrt{\sum \left(\frac{AS - FS}{AS}\right)^2} / (\text{Number of points compared})$$
.

A relatively new module has been included that simulates solute transport using particle tracking. A series of test cases are being developed but are not yet ready to be included in this version of the V&V documentation. The full set of verification tests for particle tracking will be included in the next version of this document.

Test cases for some other capabilities (such as air/water diffusion and use of unstructured grids) and some constitutive relationships (such as rock compressibility, variable thermal conductivity, and equation-of-state models) still need to be developed.

The validation effort assumes that the data will be collected to perform the validation within the LANL YMP. In particular, there are plans to collect suitable data for this validation exercise within the YMP Reactive Tracer Study Task and Dynamic Transport Task.

4.0 VERIFICATION AND VALIDATION PLAN

The V&V tests outlined in this section will apply in their entirety to any version of the code, no matter what platform is being used. The results from different platforms should be identical to within three significant digits, because the only differences in the versions should be differences in machine precision. Table 1 in Appendix B provides a summary of the FEHM requirements and a listing of which problems test them.

4.1 Testing of Thermodynamic Functions

4.1.1 Purpose

Density, viscosity, and enthalpy are strong functions of pressure (P) and temperature (T). Because FEHM is an implicit code that uses a Newton-Raphson iteration, derivatives of the thermodynamic functions with respect to P and T are also required. The equations for all water properties listed in Section 4.1.4 will be evaluated over the full range of pressure and temperature for which they were created.

The equation for the saturation line is important for the determination of the phase state of the liquid vapor system. The saturation functions will also be evaluated over the full range of pressure and temperature for which they were created.

4.1.2 Functional description

The test suite consists of a set of simple programs that call the FEHM thermodynamic functions with pressures and temperatures in the prescribed ranges. An agreement between values generated by FEHM and values in the *NBS/NRC Steam Tables* (Harr et al. 1984) with a deviation of less than 2% over the entire range of temperatures and pressures will constitute a verification of the FEHM thermodynamics functions.

4.1.3 Assumptions and limitations

The FEHM thermodynamics functions were created for a specified range of temperatures and pressures. The tests are conducted only within the specified range. Valid ranges for each function are given below under the sections entitled **Required Inputs**.

The thermodynamics functions are being tested independently of the FEHM code, so they do not test the response of the code when pressures or temperatures are out of range. For further discussion of code behavior in these cases, see the previous chapter and the FEHM document "Summary of Models and Methods" (Zyvoloski et al. 1997a).

4.1.4 Summary of test cases

4.1.4.1 Enthalpy

4.1.4.1.1 Function Tested. This test verifies that the rational polynomial expression implemented in FEHM correctly computes the enthalpy as a function of pressure and temperature.

4.1.4.1.2 Test Scope. This test is a verification test.

4.1.4.1.3 Requirements Tested. Requirement 3.3.1, "Pressure- and temperature-dependent water properties," of Chapter I is verified by this test.

4.1.4.1.4 Required Inputs. The pressures (P) and temperatures (T) at which to calculate enthalpy are required: for liquid enthalpies, the range of $0.001 \leq P \leq 110.0$ MPa and

$15 \leq T \leq 360^\circ\text{C}$; for vapor enthalpies, the range of $0.001 \leq P \leq 20.0 \text{ MPa}$ and $15 \leq T \leq 360^\circ\text{C}$.

4.1.4.1.5 Expected Outputs. Values for enthalpy from the FEHM thermodynamics functions will be output and compared to values obtained from the *NBS/NRC Steam Tables*. Values within 2% of the *Steam Tables* data will be considered acceptable.

4.1.4.2 Density

4.1.4.2.1 Function Tested. This test verifies that the rational polynomial expression implemented in FEHM correctly computes the density as a function of pressure and temperature.

4.1.4.2.2 Test Scope. This test is a verification test.

4.1.4.2.3 Requirements Tested. Requirement 3.3.1, "Pressure- and temperature-dependent water properties," of Chapter I is verified by this test.

4.1.4.2.4 Required Inputs. The pressures (P) and temperatures (T) at which to calculate density are required: for liquid densities, the range of $0.001 \leq P \leq 110.0 \text{ MPa}$ and $15 \leq T \leq 360^\circ\text{C}$; for vapor densities, the range of $0.001 \leq P \leq 20.0 \text{ MPa}$ and $15 \leq T \leq 360^\circ\text{C}$.

4.1.4.2.5 Expected Outputs. Values for density from the FEHM thermodynamics functions will be output and compared to values obtained from the *NBS/NRC Steam Tables*. Values within 2% of the *Steam Tables* data will be considered acceptable.

4.1.4.3 Compressibility (derivative of density with respect to pressure)

4.1.4.3.1 Function Tested. This test verifies that the rational polynomial expression implemented in FEHM correctly computes the compressibility (derivative of density with respect to pressure) as a function of pressure and temperature.

4.1.4.3.2 Test Scope. This test is a verification test.

4.1.4.3.3 Requirements Tested. Requirement 3.3.1, "Pressure- and temperature-dependent water properties," of Chapter I is verified by this test.

4.1.4.3.4 Required Inputs. The pressures (P) and temperatures (T) at which to calculate compressibility are required: for liquid compressibilities, the range of $0.001 \leq P \leq 110.0 \text{ MPa}$ and $15 \leq T \leq 360^\circ\text{C}$; for vapor compressibilities, the range of $0.001 \leq P \leq 20.0 \text{ MPa}$ and $15 \leq T \leq 360^\circ\text{C}$.

4.1.4.3.5 Expected Outputs. Values for compressibility from the FEHM thermodynamics functions will be output and compared to values obtained from the *NBS/NRC Steam Tables*. Compressibility is a commonly used property of the fluid but

does not appear directly in the equations that are solved and does not affect the solution. The compressibility is not directly derived from the *Steam Tables* data but is computed from the derivative of the density function. Therefore, values within 10% of the *Steam Tables* data will be considered acceptable.

4.1.4.4 Viscosity

4.1.4.4.1 Function Tested. This test verifies that the rational polynomial expression implemented in FEHM correctly computes the viscosity as a function of pressure and temperature.

4.1.4.4.2 Test Scope. This test is a verification test.

4.1.4.4.3 Requirements Tested. Requirement 3.3.1, "Pressure- and temperature-dependent water properties," of Chapter I is verified by this test.

4.1.4.4.4 Required Inputs. The pressures (P) and temperatures (T) at which to calculate viscosity are required: for liquid viscosities, the range of $0.001 \leq P \leq 110.0$ MPa and $15 \leq T \leq 360$ °C; for vapor viscosities, the range of $0.001 \leq P \leq 20.0$ MPa and $15 \leq T \leq 360$ °C.

4.1.4.4.5 Expected Outputs. Values for viscosity from the FEHM thermodynamics functions will be output and compared to values obtained from the *NBS/NRC Steam Tables*. Values within 2% of the *Steam Tables* data will be considered acceptable.

4.1.4.5 Saturation pressure and temperature

4.1.4.5.1 Function Tested. This test verifies that the rational polynomial expression implemented in FEHM correctly computes the pressure as a function of saturation temperature and the temperature as a function of saturation pressure.

4.1.4.5.2 Test Scope. This test is a verification test.

4.1.4.5.3 Requirements Tested. Requirement 3.3.2, "Properties of air and air/water vapor mixtures," of Chapter I is verified by this test.

4.1.4.5.4 Required Inputs. The temperatures (T) at which to calculate saturation pressure and the pressures (P) for which to calculate saturation temperature are required: in the range of $0.00123 \leq P \leq 14.59410$ MPa and $10 \leq T \leq 340$ °C.

4.1.4.5.5 Expected Outputs. Values for saturation pressure and temperature from the FEHM thermodynamics functions will be output and compared to values obtained from the *NBS/NRC Steam Tables*. Values within 2% of the *Steam Tables* data will be considered acceptable.

4.2 Test of Heat Conduction

4.2.1 Purpose

Though simple heat-conduction simulations without flow are not used in the modeling studies of Yucca Mountain, heat transfer is an important process in many calculations, including potential repository-heating calculations. Furthermore, it is convenient to use the analytical solutions available for 2-D and 3-D heat conduction in solids. The solutions give an excellent check on the purely geometric aspects of the code as well as the finite-element representation of second-order partial differential equations. The code will be checked against both 2-D and 3-D analytical solutions with regular grid spacing for triangular, rectangular, prism, brick, tetrahedral, and mixed elements. All solutions will be for linear (constant parameter) problems.

4.2.2 Functional description

The test suite consists of a set of simulations, with heat conduction only, that model the same problem using different finite-element meshes. In addition to demonstrating that the heat-conduction problem has been correctly formulated, the test suite will demonstrate that the various element types have been correctly implemented.

4.2.3 Assumptions and limitations

The analytical solutions for 2-D and 3-D heat conduction are provided by Carslaw and Jaeger (1959). For two-dimensional heat conduction in a rectangle, the analytical solution takes the form:

$$T = T_s + \frac{16(T_0 - T_s)}{\pi^2} \left(\sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \frac{(-1)^{m+n}}{(2m+1)(2n+1)} \cos \frac{(2m+1)\pi x}{2a} \cos \frac{(2n+1)\pi y}{2b} e^{-\alpha_{m,n} t} \right),$$

where $\alpha_{m,n} = \frac{\kappa\pi^2}{4} \left[\frac{(2m+1)^2}{a^2} + \frac{(2n+1)^2}{b^2} \right]$ and the region is taken to be $-a < x < a, -b < y < b$.

Extended to three-dimensional heat conduction in a cube:

$$T = T_s + \frac{64(T_0 - T_s)}{\pi^3} \left(\sum_{l=0}^{\infty} \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \frac{(-1)^{l+m+n}}{(2l+1)(2m+1)(2n+1)} \cos \frac{(2l+1)\pi x}{2a} \cos \frac{(2m+1)\pi y}{2b} \cos \frac{(2n+1)\pi z}{2c} e^{-\alpha_{l,m,n} t} \right),$$

where $\alpha_{l,m,n} = \frac{\kappa\pi^2}{4} \left[\frac{(2l+1)^2}{a^2} + \frac{(2m+1)^2}{b^2} + \frac{(2n+1)^2}{c^2} \right]$ and the rectangular region is taken to be $-a < x < a, -b < y < b, -c < z < c$.

Heat conduction in a solid 1-meter square/cube with an initial temperature $T_0 = 200^\circ\text{C}$ is modeled after a surface temperature $T_s = 100^\circ\text{C}$ is imposed at time $t = 0$. Due to symmetry, only a quarter of the square, or an eighth of the cube (0.5 meters on a side), needs to be modeled (see Fig. 1). Table 22

summarizes the rock properties and problem dimensions used for the heat-conduction problem.

Figure 1. Schematic diagrams of 2-D and 3-D heat-conduction problems.

Table 22. Input parameters for the 2-D and 3-D heat-conduction problems		
Parameter	Symbol	Value
Rock thermal conductivity	κ_r	$2.7 \frac{\text{W}}{\text{m} \cdot \text{K}}$
Rock density	ρ_r	2700 kg/m^3
Rock specific heat	C_r	$1000 \frac{\text{J}}{\text{kg} \cdot \text{K}}$
Rock thermal diffusivity	$\kappa = \frac{\kappa_r}{\rho_r C_r}$	$10^{-6} \text{ m}^2/\text{s}$
Width	a	0.5 m
Length	b	0.5 m
Height	c	0.5 m
Node spacing	$\Delta x, \Delta y, \Delta z$	0.05 m
Time step	Δt	0.005 days
Total elapsed time	t	4 days (2-D) 3 days (3-D)
Initial temperature	T_0	200°C
Boundary conditions: At $x, y, z = 0.5$ m, $T_s(t) = 100^\circ\text{C}$		

4.2.4 Summary of test cases

4.2.4.1 2-D heat conduction in a square

4.2.4.1.1 Function Tested. This test verifies that FEHM correctly models two-dimensional heat conduction. It also verifies that the 2-D finite-element representation of 3-node triangles (triangular-element meshes), 4-node quadrilaterals (rectangular-element meshes), mixed-element meshes (containing both triangular and rectangular elements), and refined-element meshes (containing rectangular and trapezoidal elements) have been correctly implemented (see Fig. 2).

Figure 2. Geometric configurations tested by the 2-D heat-conduction problem.

4.2.4.1.2 Test Scope. This test case is a verification test.

4.2.4.1.3 Requirements Tested. Requirements 3.1, "Finite-Element Coefficient Generation," 3.2, "Formulate Transient Equations" (specifically Section 3.2.1), 3.4, "Compute Solution to Transient Equations," and 3.5, "Provide Input/Output Data Files," of Chapter I are verified by this test.

4.2.4.1.4 Required Inputs. Input is provided in the following files:

- *heat2d.in*: basic input data file used in conjunction with the following geometry data files:
- *heat2d.geom.2d_tri*: 3-node triangles (121 nodes, 200 elements),

- *heat2d.geom.2d_quad*: 4-node quadrilaterals (121 nodes, 100 elements),
- *heat2d.geom.2d_mix*: mixed elements, 3-node triangles and 4-node quadrilaterals (121 nodes, 104 elements), or
- *heat2d.geom.2d_ref*: refined elements, 4-node quadrilaterals with refinement about the node at $x = y = 0$ m (127 nodes, 104 elements).

4.2.4.1.5 Expected Outputs. Values from FEHM for temperature versus time at the center of the square ($x = y = 0$ m) and values for temperature versus position ($x = y$) at a specified time (time = 0.25 days) will be output and compared to the analytical solution. Values within 5% of the analytical solution will be considered acceptable.

4.2.4.2 3-D heat conduction in a cube

4.2.4.2.1 Function Tested. This test verifies that FEHM correctly models three-dimensional heat conduction. It also verifies that the finite-element representation of 3-D, 6-node triangular prisms (prism elements), 8-node quadrilateral polyhedrons (brick elements), 4-node tetrahedrals, mixed-element meshes (containing both triangular prisms and quadrilateral polyhedrons), and refined-element meshes (containing quadrilateral polyhedrons and trapezoidal polyhedrons) have been correctly implemented (see Fig. 3). In addition, the finite-volume option, in which the code subdivides brick elements into tetrahedrals, is tested.

4.2.4.2.2 Test Scope. This test case is a verification test.

4.2.4.2.3 Requirements Tested. Requirements 3.1, "Finite-Element Coefficient Generation," 3.2, "Formulate Transient Equations" (specifically Section 3.2.1), 3.4, "Compute Solution to Transient Equations," and 3.5, "Provide Input/Output Data Files," of Chapter I are verified by this test.

4.2.4.2.4 Required Inputs. Problem input is provided in the following files:

- *heat3d.in*: basic input data file used in conjunction with the following geometry data files:
- *heat3d.geom.3d_tri*: 6-node triangular prisms (1331 nodes, 2000 elements),
- *heat3d.geom.3d_quad*: 8-node quadrilateral polyhedrons (1331 nodes, 1000 elements),
- *heat3d.geom.3d_tets*: 4-node tetrahedrals (1331 nodes, 6000 elements),

Figure 3. Geometric elements tested by the 3-D heat-conduction problem.

- *heat3d.geom.3d_mix*: mixed elements, 6-node triangular prisms and 8-node quadrilateral polyhedrons (1331 nodes, 1020 elements), or
- *heat3d.geom.3d_ref*: refined elements, 8-node quadrilateral polyhedrons with refinement about node at $x = y = 0$ m for $z = 0$ to 0.5 m (1364 nodes, 1020 elements); and
- *heat3d.finv.in*: basic input data file using the finite-volume option used in conjunction with the following geometry data files:
- *heat3d.geom.3d_quad* or
- *heat3d.geom.3d_ref*.

4.2.4.2.5 Expected Outputs. Values from FEHM for temperature versus time at the center of the cube ($x = y = z = 0$ m) and values for temperature versus position ($x = y = z$) at a specified time (time = 0.25 days) will be output and compared to the analytical solution. Values within 5% of the analytical solution will be considered acceptable.

4.3 Test of Temperature in a Wellbore

4.3.1 Purpose

The ability to model temperature changes in a wellbore is important to the interpretation of temperature surveys. Ramey (1962) has developed a semianalytical technique for predicting the thermal drawdown in a wellbore. Comparison with this solution will help verify that the code is capable of analyzing temperature logs and, more generally, of handling a thermal-conduction problem coupled to advective heat transport.

4.3.2 Functional description

The test suite consists of a simulation of fluid injection into a wellbore. In addition to demonstrating that the heat- and mass-transfer problem has been correctly formulated, the test suite will demonstrate that the 2-D radial geometry has been correctly implemented.

4.3.3 Assumptions and limitations

Fluid injection at constant temperature, T_{inj} , into a wellbore is modeled (Fig. 4). Flow is confined to the wellbore, i.e., there is no flow between the wellbore and the surrounding rock. The semianalytical solution is given by

$$T_f(z,t) = b + az - aA + (T_{inj} - b + aA)e^{-\frac{z}{A}},$$

$$\text{where } A = \frac{qcf(t)}{2\pi\kappa} \text{ and } f(t) = \frac{1}{\frac{4}{\pi^2} \int_0^\infty \frac{e^{-au^2t}}{u(J_0^2(r_w u) + Y_0^2(r_w u))} du}.$$

J_0 and Y_0 are Bessel functions of the first and second kind, of order 0, respectively. The initial temperature distribution in the medium is given by a linear geothermal gradient $T_r = b + az$, where b is the surface rock temperature and a is the geothermal gradient. Although the Ramey solution models a semi-infinite reservoir in the radial direction, for the FEHM model, the reservoir radius has been set to 40 m. Table 23 defines the input parameters used for FEHM and the Ramey analytical solution.

4.3.4 Summary of test cases

4.3.4.1 Constant-temperature injection into a wellbore

4.3.4.1.1 Function Tested. This test verifies that FEHM has correctly implemented the heat- and mass-transfer problem and 2-D radial geometry.

4.3.4.1.2 Test Scope. This test case is a verification test.

Figure 4. Schematic drawing of the problem geometry and boundary conditions for the temperature-in-a-wellbore problem.

4.3.4.1.3 Requirements Tested. Requirements 3.1, "Finite-Element Coefficient Generation," 3.2, "Formulate Transient Equations" (specifically Sections 3.2.2 and 3.2.6), 3.3, "Apply Constitutive Relationships" (specifically Section 3.3.1), 3.4, "Compute Solution to Transient Equations," and 3.5, "Provide Input/Output Data Files," of Chapter I are verified by this test.

4.3.4.1.4 Required Inputs. Problem input is provided in the following files:

- *ramey.in*: basic input data and
- *ramey.geom*: geometry data (1010 nodes, 900 elements).

4.3.4.1.5 Expected Outputs. Values from FEHM for temperature versus time at fixed depth ($d = 1000$ and 2000 m) and values for temperature versus depth ($d = 0$ to 2000 m) at a specified time ($t = 25$ days) will be output and compared to the analytical solution. Values within 5% of the analytical solution will be considered acceptable.

Table 23. Input parameters for the temperature-in-a-wellbore problem

Parameter	Symbol	Value
Rock thermal conductivity	κ_r	$2.7 \frac{\text{W}}{\text{m} \cdot \text{K}}$
Rock density	ρ_r	2700 kg/m^3
Rock specific heat	C_r	$1000 \frac{\text{J}}{\text{kg} \cdot \text{K}}$
Rock thermal diffusivity	$\alpha_r = \frac{\kappa_r}{\rho_r C_r}$	$10^{-6} \text{ m}^2/\text{s}$
Rock (matrix) permeability	k	10^{-20} m^2
Porosity	f	0
Fluid heat capacity	C_f	$4200 \frac{\text{J}}{\text{kg} \cdot \text{K}}$
Wellbore radius	r_w	0.09808 m
Radial extent	r	40 m
Node spacing (radial)	Δr	0.19616 - 17.25495 m
Well depth	z	2000 m
Node spacing (vertical)	Δz	20 m
Surface rock temperature	b	20°C
Geothermal gradient	a	0.03°C/m
Injection rate	q	0.5 kg/s
Injection temperature	T_{inj}	20°C
Time step	Δt	0.001 - 1 days
Total elapsed time	t	25 days
Initial temperature distribution (T in °C, z in m): $T(z) = 20 + 0.03 z$ for $r = 0 - 40 \text{ m}$		
Boundary conditions: At $r = 0 \text{ m}$, $z = 0 \text{ m}$, $q = 0.5 \text{ kg/s}$, $T_{inj} = 20^\circ\text{C}$ At $r = 0 \text{ m}$, $z = 2000 \text{ m}$, $P(t) = 5 \text{ MPa}$		

4.4 Test of Pressure Transient Analysis

4.4.1 Purpose

Properties of underground reservoirs are often determined by pressure tests. Theis (1935) developed a solution for radial flow to a well in the form of pressure as a function of time and the spatial coordinates. Comparison with this solution will help demonstrate that the pressure equation (the conservation of mass with Darcy's law) is implemented correctly.

4.4.2 Functional description

The test suite consists of a simulation of 1-D radial flow into an infinite aquifer. In addition to demonstrating that the transient pressure equation has been correctly formulated, the test suite will demonstrate that the radial geometry has been correctly implemented.

4.4.3 Assumptions and limitations

Injection into a centrally located well at a constant volumetric rate, q , is modeled. The well (modeled as a line source) is assumed to be situated in a porous medium of infinite radial extent. The analytical solution (from Matthews and Russell 1967) is given by

$$p(r,t) = p_i - \frac{q\mu}{2\pi kh} \left[-\frac{1}{2} E_i \left(-\frac{\phi\mu cr^2}{4kt} \right) \right],$$

where the exponential integral function is $-E_i(-x) = \int_x^\infty \frac{e^{-u}}{u} du$.

Figure 5 shows the problem geometry and boundary conditions. This problem is isothermal. Input parameters defining the problem are given in Table 24.

Figure 5. Schematic drawing of the problem geometry and boundary conditions for the transient pressure problem.

Table 24. Input parameters for the transient pressure problem

Parameter	Symbol	Value
Reservoir permeability in radial direction	k	10^{-14} m^2
Reservoir porosity	ϕ	0.4
Fluid compressibility	c	$5.06 \cdot 10^{-4} \text{ MPa}^{-1}$
Fluid viscosity	μ	$5.48 \cdot 10^{-4} \text{ Pa}\cdot\text{s}$
Reservoir thickness	h	100 m
Node spacing (vertical)	Δh	100 m
Reservoir length (radial)	r	0 - 1000 m
Node spacing (radial)	Δr	0.00144 - 107 m
Flow rate	q	$2.22 \cdot 10^{-4} \text{ kg/s}$
Initial pressure	p_i	1 MPa
Temperature (isothermal)	T	50°C
Time step	Δt	300 s
Total elapsed time	t	1 day
Boundary conditions: $p \rightarrow p_i$ as $r \rightarrow \infty$ $\lim_{r \rightarrow 0} r \frac{\partial p}{\partial r} = \frac{q\mu}{2\pi kh} \text{ (constant flow at } r = 0, \text{ line source)}$		

4.4.4 Summary of test cases

4.4.4.1 Radial flow from a well

4.4.4.1.1 Function Tested. This test verifies that FEHM has correctly implemented the pressure equations, i.e., the conservation of mass with Darcy's law.

4.4.4.1.2 Test Scope. This test case is a verification test.

4.4.4.1.3 Requirements Tested. Requirements 3.1, "Finite-Element Coefficient Generation," 3.2, "Formulate Transient Equations" (specifically Sections 3.2.2 and 3.2.6), 3.4, "Compute Solution to Transient Equations," and 3.5, "Provide Input/Output Data Files," of Chapter I are verified by this test.

4.4.4.1.4 Required Inputs. Problem input is provided in the following file:

- *theis.in*: basic input and geometry data (202 nodes, 100 elements).

4.4.4.1.5 Expected Outputs. Values from FEHM, for pressure versus time, at fixed radii ($r = 0.00144$ and 3.44825 m), and values for pressure versus radius ($r = 0$ to 1000 m), at a specified time ($t = 1$ day), will be output and compared to the analytical solution. Values within 5% of the analytical solution will be considered acceptable.

4.5 Test of Infiltration into a One-dimensional, Layered, Unsaturated Medium

4.5.1 Purpose

Modeling infiltration into an unsaturated medium can be performed by implementing either the equivalent-continuum method (ECM) or the double-porosity/double-permeability method (DKM). The ECM provides a lumped set of properties for the material that are derived from the separate matrix and fracture properties along with hydrologic conditions such as saturation and pressure. The DKM considers the fractures as a continuous medium and the matrix as another continuous medium and provides for conductance between the two. See the FEHM document "Summary of Methods and Models" (Zyvoloski et al. 1997a, Section 8.2) for more details of the double-porosity/double-permeability method. The DKM requires twice as many finite-element nodes and hence takes longer to run than the ECM. Both methods use the same set of van Genuchten capillary-pressure model parameters to describe the hydrologic properties. The two methods are often compared with each other to assess whether the additional computational burden associated with the DKM is necessary to capture behavior such as fast flow paths in fractures, which are smoothed out in the composite-property model of the ECM. This set of tests verifies that each method, the ECM and the DKM, are implemented properly.

4.5.2 Functional description

The test problem, described by Ho (1995a, 1995b), consists of simulations of infiltration into a one-dimensional column. The column is a transect through a system of four stratigraphic units, each characterized by a unique set of parameters describing the matrix and fracture properties. The stratigraphic system is a representation of the lithologic layering at Yucca Mountain. The four units are the Tiva Canyon welded tuff (TCw), the Paintbrush nonwelded tuff (PTn), the Topopah Springs welded tuff (TSw), and the Calico Hills nonwelded vitrophere (CHnv). A schematic of the thicknesses and layering of the four units considered is shown in Fig. 6. The properties for these four units were taken from YMP total system performance assessment of 1993 (Wilson 1994) and are located in the required inputs files. Key aspects of this data set include matrix intrinsic permeabilities and matrix residual saturations, each of which span four orders of magnitude over the various units.

The test will demonstrate that the equivalent-continuum method and the double-porosity/double-permeability method have been correctly implemented through comparison with simulations performed with TOUGH2, another well-documented model capable of solving this problem (Pruess 1991).

Figure 6. Schematic drawing of the problem geometry for the test of the one-dimensional infiltration problem.

4.5.3 Assumptions and limitations

Infiltration of 4 mm/yr is applied at the top of the system. For the DKM simulations, it is applied to the fracture nodes only. The bottom boundary for all tests is assumed to be the water table, so full saturation is set there. The TOUGH2 simulations with which FEHM will be compared were run at Sandia National Laboratories using TOUGH2 - version 1.1 (April 1993). This is an isothermal air-water problem. Input parameters defining the problem are given in Table 25.

4.5.4 Summary of test cases

4.5.4.1 Test of infiltration into a one-dimensional, layered, unsaturated medium using the equivalent-continuum method (ECM)

4.5.4.1.1 Function Tested. This test verifies that FEHM has correctly implemented for simulations of infiltration into a one-dimensional, layered, unsaturated medium using ECM.

4.5.4.1.2 Test Scope. This test case is a verification test.

Table 25. Input parameters for the one-dimensional infiltration problem		
Parameter	Symbol	Value
Fracture permeability		
TCw	k_f	$2.04 \cdot 10^{-18} \text{ m}^2$
PTn		$2.51 \cdot 10^{-14} \text{ m}^2$
TSw		$2.09 \cdot 10^{-18} \text{ m}^2$
CHnv		$1.10 \cdot 10^{-16} \text{ m}^2$
Matrix permeability		
TCw	k_m	$4.06 \cdot 10^{-9} \text{ m}^2$
PTn		$7.14 \cdot 10^{-9} \text{ m}^2$
TSw		$4.57 \cdot 10^{-9} \text{ m}^2$
CHnv		$6.53 \cdot 10^{-9} \text{ m}^2$
Fracture porosity (volume fraction for fracture node)		
TCw	$\phi_f (V_f)$	$2.93 \cdot 10^{-4}$
PTn		$9.27 \cdot 10^{-5}$
TSw		$2.43 \cdot 10^{-4}$
CHnv		$1.11 \cdot 10^{-4}$
Matrix porosity		
TCw	ϕ_m	0.087
PTn		0.421
TSw		0.139
CHnv		0.331
Matrix-node length scale		
TCw	L_{fl}	0.18 m
PTn		0.64 m
TSw		0.21 m
CHnv		0.46 m
Column width	w	10 m
Node spacing (horizontal)	Δw	10 m
Column height (elevation)	h	0 - 530 m
Node spacing (vertical) [‡]	Δh	5 m
Reference pressure	P_r	0.1 MPa
Reference temperature	T_r	20°C
Maximum saturation	S_{lmax}	1.0
Fracture residual saturation	$S_{lr,f}$	0.03

Table 25. Input parameters for the one-dimensional infiltration problem (continued)

Parameter	Symbol	Value
Matrix residual saturation		
TCw	$S_{lr,m}$	0.0212
PTn		0.154
TSw		0.0453
CHnv		0.0968
van Genuchten model parameters for the fracture		
Inverse of air entry pressure		
TCw	$\alpha_{G,f}$	12.05 m ⁻¹
PTn		2.5 m ⁻¹
TSw		11.96 m ⁻¹
CHnv		2.5 m ⁻¹
Power in formula		
TCw	n_f	3.0
PTn		3.0
TSw		3.0
CHnv		3.0
van Genuchten model parameters for the matrix		
Inverse of air entry pressure		
TCw	$\alpha_{G,m}$	0.00715 m ⁻¹
PTn		0.371 m ⁻¹
TSw		0.0133 m ⁻¹
CHnv		0.0273 m ⁻¹
Power in formula		
TCw	n_m	1.62
PTn		2.37
TSw		1.8
CHnv		2.46
Initial fracture saturation	$S_{lo,f}$	0.5
Initial matrix saturation		
TCw	$S_{lo,m}$	0.95
PTn		0.31
TSw		0.95
CHnv		0.85
Time step	Δt	1 - 1*10 ⁻⁸ days
Total elapsed time	t	1*10 ⁻⁹ days
Boundary conditions: At $h = 530$ m $q = 4$ mm/yr At $h = 0$ m $S = 1.0$		
‡ For the FEHM simulation, an additional node was added at each material interface to facilitate comparison with TOUGH2, which uses cell-centered elements, whereas FEHM uses node-centered elements.		

4.5.4.1.3 Requirements Tested. Requirements 3.1, "Finite-Element Coefficient Generation," 3.2, "Formulate Transient Equations" (specifically Sections 3.2.2 and 3.2.6), 3.3, "Apply Constitutive Relationships" (specifically Section 3.3.4), 3.4, "Compute Solution to Transient Equations," and 3.5, "Provide Input/Output Data Files," of Chapter I are verified by this test.

4.5.4.1.4 Required Inputs. Problem input is provided in the following files:

- *infiltration.ecm.in*: basic input data, case 1, and
- *infiltration.geom*: geometry data used for the above cases.

4.5.4.1.5 Expected Outputs. Values from FEHM for saturation versus elevation will be output, nondimensionalized, and compared to the TOUGH2 solution. A root-mean-square error of the difference between the two simulations less than or equal to 0.05 will be considered acceptable.

4.5.4.2 Test of infiltration into a one-dimensional, layered, unsaturated medium using the double-porosity/double-permeability method (DKM)

4.5.4.2.1 Function Tested. This test verifies that FEHM has been correctly implemented for simulations of infiltration into a one-dimensional, layered, unsaturated medium using DKM.

4.5.4.2.2 Test Scope. This test case is a verification test.

4.5.4.2.3 Requirements Tested. Requirements 3.1, "Finite-Element Coefficient Generation," 3.2, "Formulate Transient Equations" (specifically Sections 3.2.2 and 3.2.6), 3.3, "Apply Constitutive Relationships" (specifically Sections 3.3.4 and 3.3.8), 3.4, "Compute Solution to Transient Equations," and 3.5, "Provide Input/Output Data Files," of Chapter I are verified by this test.

4.5.4.2.4 Required Inputs. Problem input is provided in the following files:

- *infiltration.dpm.in*: basic input data, case 2, and
- *infiltration.geom*: geometry data used for the above cases.

4.5.4.2.5 Expected Outputs. Values from FEHM for saturation versus elevation will be output, nondimensionalized, and compared to the TOUGH2 solution. A root-mean-square error of the difference between the two simulations less than or equal to 0.05 will be considered acceptable.

4.6 Test of Vapor Extraction from an Unsaturated Reservoir

4.6.1 Purpose

The ability to model vapor/gas transport in unsaturated media is important to the design of vapor-extraction systems and interpretation of their performance. Analytical solutions of steady-state gas flow to a soil vapor-extraction well in the unsaturated zone have been described by Shan et al. (1992). Comparison with this solution will help verify that vapor/gas transport has been correctly implemented in FEHM.

4.6.2 Functional description

The test suite consists of two simulations of steady, 2-D radial soil-vapor flow to a well in an unsaturated reservoir. The first case uses an isotropic permeability model, whereas the second case models an anisotropic reservoir. In addition to demonstrating that the gas-flow problem has been correctly formulated for isotropic and anisotropic permeability models, the test suite will demonstrate that the 2-D radial coordinate geometry has been correctly implemented.

4.6.3 Assumptions and limitations

The analytical solution for pressure for this test case is expressed as an infinite series:

$$P = \frac{\bar{q}}{4\pi\alpha_r} \left[\ln \left(\frac{a-z + [\hat{r}^2 + (a-z)^2]^{-1/2}}{b-z + [\hat{r}^2 + (b-z)^2]^{-1/2}} \cdot \frac{b+z + [\hat{r}^2 + (b+z)^2]^{-1/2}}{a+z + [\hat{r}^2 + (a+z)^2]^{-1/2}} \right) - \sum_{n=1}^{\infty} (-1)^n \ln \left(\frac{a+z+2nh + [\hat{r}^2 + (a+z+2nh)^2]^{-1/2}}{b+z+2nh + [\hat{r}^2 + (b+z+2nh)^2]^{-1/2}} \cdot \frac{a+z-2nh + [\hat{r}^2 + (a+z-2nh)^2]^{-1/2}}{b+z-2nh + [\hat{r}^2 + (b+z-2nh)^2]^{-1/2}} \cdot \frac{-a+z+2nh + [\hat{r}^2 + (-a+z+2nh)^2]^{-1/2}}{-b+z+2nh + [\hat{r}^2 + (-b+z+2nh)^2]^{-1/2}} \cdot \frac{-a+z-2nh + [\hat{r}^2 + (-a+z-2nh)^2]^{-1/2}}{-b+z-2nh + [\hat{r}^2 + (-b+z-2nh)^2]^{-1/2}} \right) \right],$$

$$\text{where } \bar{q} = \frac{2P_a q_m}{(a-b)\phi\rho_g}, \alpha_r = \frac{k_r P_a}{\phi\mu_g}, \hat{r} = \left(\frac{k_z}{k_r} \right)^{1/2} r,$$

r is the radial distance, z is the vertical distance, h is the depth to the water table (impermeable boundary), and a and b are the depths to the bottom and top of the open wellbore interval, respectively. A sensitivity study of the number of terms required for the solution to achieve a precision of 10^{-3} Pa shows that no more than 50 terms are needed.

The geometry and boundary conditions are shown in Fig. 7. The upper surface is at atmospheric pressure and the remaining edges are impermeable; there are no flow boundaries, with the exception of the extraction wellbore. The problem is isothermal. Values of the analytical solution are inaccurate in the region surrounding the extraction wellbore ($r \leq 0.05$ m, $2.8 \leq z \leq 7.2$ m), so they are excluded from the results used for comparison. Table 26 lists the input parameters for the vapor-extraction problem. The solution is verified by comparison of FEHM results to the analytical solution.

Figure 7. Schematic diagram of the geometry and boundary conditions for the vapor-extraction problem.

Table 26. Input parameters for the vapor-extraction problem		
Parameter	Symbol	Value
Reservoir permeability		
Isotropic case	k_r, k_z	10^{-11} m^2
Anisotropic case -radial	k_r	10^{-11} m^2
Anisotropic case -vertical	k_z	10^{-12} m^2
Reservoir porosity	ϕ	0.4
Reservoir length	r	0 - 30 m

Table 26. Input parameters for the vapor-extraction problem (continued)

Node spacing (radial)	Δr	0.0001 - 1 m
Reservoir thickness (elevation)	h	0 - 10 m
Node spacing (vertical)	Δh	0.5 m
Extraction interval, bottom	a	3 m
Extraction interval, top	b	7 m
Ambient (reference) temperature	T_a	10°C
Ambient pressure	P_a	0.101325 MPa
Initial pressure	P_0	0.101325 MPa
Initial saturation	S_0	0.05
Residual liquid saturation	S_{lr}	0.10
Maximum liquid saturation	S_{lmax}	0.99
van Genuchten model parameters		
Inverse of air entry pressure	α_G	0.005 m ⁻¹
Power in formula	n	1.8
Gas density	ρ_g	1.24 kg/m ³
Gas viscosity	μ_g	1.76 x 10 ⁻⁵ Pa·s
Extraction rate		
Isotropic case	q_m	0.0825 kg/s
Anisotropic case		0.05 kg/s
Time step	Δt	0.001 - 75 days
Total elapsed time		
Isotropic case	t	365 days
Anisotropic case		730 days
Boundary conditions: At $z = 10$ m $P = 0.101325$ MPa, $S = 0.05$ At $r = 0$ m, $3 \leq z \leq 7$ m $q = q_m$ (Line sink wellbore, z positive upwards)		

4.6.4 Summary of test cases

4.6.4.1 Vapor extraction from an unsaturated reservoir

4.6.4.1.1 Function Tested. This test verifies that FEHM has correctly implemented the gas-flow option of the code for radial flow.

4.6.4.1.2 Test Scope. This test case is a verification test.

4.6.4.1.3 Requirements Tested. Requirements 3.1, "Finite-Element Coefficient Generation," 3.2, "Formulate Transient Equations" (specifically Sections 3.2.3 and 3.2.6), 3.3, "Apply Constitutive Relationships" (specifically Sections 3.3.2 and 3.3.4), 3.4, "Compute Solution to Transient Equations," and 3.5, "Provide Input/Output Data Files," of Chapter I are verified by this test.

4.6.4.1.4 Required Inputs. Problem input is provided in the following files:

- *vapextract_iso.in*: basic input data, isotropic case,
- *vapextract_aniso.in*: basic input data, anisotropic case, and
- *vapextract.geom*: geometry data used for the above cases.

4.6.4.1.5 Expected Outputs. Values from FEHM for the steady-state vapor pressure at each node (reached after 365 days for the isotropic case, 730 days for the anisotropic case) will be output and compared to the analytical solution from Shan et al. (1992). Values within 5% of the analytical solution or a root-mean-square error of the difference between the two simulations less than or equal to 0.01 will be considered acceptable.

4.7 Test of Dual Porosity

4.7.1 Purpose

The dual-porosity formulation is a computationally efficient way to model flow in a porous media with high-permeability fractures embedded in low-permeability matrix material. It has previously been shown by Moench (1984) that dual-porosity flow can explain some of the well test data at Yucca Mountain. Warren and Root (1963) provide an analytical solution for dual-porosity flow to a wellbore. This test will check the pressure solution for the dual-porosity coding in FEHM.

4.7.2 Functional description

The test suite consists of a set of simulations of dual-porosity flow to a wellbore. It will demonstrate that the dual-porosity formulation has been correctly implemented.

4.7.3 Assumptions and limitations

Warren and Root have defined the dimensionless pressure drop as

$$\psi_f(1, \tau) \approx \frac{1}{2} \left\{ \ln \tau + 0.80908 + Ei \left[\frac{-\lambda \tau}{\omega(1-\omega)} \right] - Ei \left[\frac{-\lambda \tau}{1-\omega} \right] \right\},$$

$$\text{where } \tau = \frac{\bar{k}_f t}{\phi_m c_m + \phi_f c_f},$$

$$\bar{k}_f = \sqrt{k_{fx} k_{fy}},$$

$$\lambda = \frac{\alpha k_m r_w^2}{\bar{k}_f},$$

$$\omega = \frac{\phi_f c_f}{\phi_m c_m + \phi_f c_f},$$

and Ei is the exponential integral function (see Section 4.4.3). In this solution, τ is dimensionless time, $\bar{k}_f$ is the effective permeability of the anisotropic medium, λ is a measure of the size of the matrix region, ω represents the strength of coupling between the fracture and the matrix, and α is a characteristic dimension.

Figure 8 illustrates the problem geometry and boundary conditions. The input parameters are defined in Table 27. The analytical solution uses a steady-state approximation for the matrix flow (only one matrix node exists per fracture node), so no transient effects are possible in the matrix. The FEHM dual-porosity implementation uses a transient approximation for the matrix material (two matrix nodes exist for each fracture node), so crude transient responses are possible because of flow between two matrix nodes. See the FEHM document "Methods and Models" (Zyvoloski et al. 1997a, Section 8.2) for more details and a description of the model

parameters (L_f and V_f). The steady-state approximation is known to be inaccurate at small times (see Warren and Root 1963, p. 248) and is only valid for τ greater than ~ 100 .

Figure 8. Schematic diagram of the geometry and boundary conditions for the dual-porosity problem.

Table 27. Input parameters for the dual-porosity problem			
Parameter	Symbol	Value	
Permeability			
fracture			$0.4 \times 10^{-12} \text{ m}^2$
matrix {	k_f	(1)	$1.904 \times 10^{-16} \text{ m}^2$
		(2)	$1.904 \times 10^{-13} \text{ m}^2$
		(3)	$1.194 \times 10^{-14} \text{ m}^2$
Porosity			
fracture			1.0
matrix {	ϕ_f	(1)	0.06081
		(2)	0.6081
		(3)	0.47
Volume fraction			
fracture node {	V_f	(1)(2)	0.006711409
		(3)	0.000476417
first matrix node {	V_{f1}	(1)(2)	0.335570470
		(3)	0.333492139
Number in () denotes for which case that value was used.			

Table 27. Input parameters for the dual-porosity problem (continued)		
Parameter	Symbol	Value
Length scale $\begin{cases} (1)(2) \\ (3) \end{cases}$	L_{f0}	0.10 0.01
Compressibility (fracture and matrix)	$c_f c_m$	5.503e-4 MPa ⁻¹
Flow rate	q	0.1 kg/s
Viscosity	μ	1.0021e-3 Pa•s
Reference temperature	T	20°C
Initial pressure	P_0	2.0 MPa
Wellbore radius	r_w	0.17528 m
Reservoir length	r	0 - 1000 m
Node spacing (radial) [average of graded mesh 1.0 m]	Δr	0.07 - 10 m
Reservoir height	h	2 m
Node spacing (vertical)	Δh	2 m
Time step $\begin{cases} (1) \\ (2)(3) \end{cases}$	Δt	1.0*10 ⁻⁸ - 0.01 days 2.0*10 ⁻⁷ - 0.01 days
Total elapsed time $\begin{cases} (1) \\ (2)(3) \end{cases}$	t	0.1 days 0.2 days
Boundary conditions: At $r = r_w = 0.17528$ m $q = 0.1$ kg/s At $r = 1000$ m No flow boundary (Sufficiently large to approximate semi-infinite reservoir)		
Number in () denotes for which case that value was used.		

4.7.4 Summary of test cases

4.7.4.1 Dual-porosity problem

4.7.4.1.1 **Function Tested.** This test verifies that FEHM has correctly implemented the dual-porosity formulation.

4.7.4.1.2 **Test Scope.** This test case is a verification test.

4.7.4.1.3 **Requirements Tested.** Requirements 3.1, "Finite-Element Coefficient Generation," 3.2, "Formulate Transient Equations"

(specifically Sections 3.2.2 and 3.2.6), 3.3, "Apply Constitutive Relationships" (specifically Sections 3.3.1 and 3.3.7), 3.4, "Compute Solution to Transient Equations," and 3.5, "Provide Input/Output Data Files," of Chapter I are verified by this test.

4.7.4.1.4 Required Inputs. Problem input is provided in the following files:

- *dual1.in*: basic input data, case 1,
- *dual2.in*: basic input data, case 2,
- *dual3.in*: basic input data, case 3, and
- *dual.geom*: geometry data used for the above cases.

4.7.4.1.5 Expected Outputs. Values from FEHM for pressure versus time at the wellbore fracture node, $r = 0.1398$ (i.e., interior node closest to $r_w = 0.17528$), will be output, nondimensionalized, and compared to the Warren and Root analytical solution. Values within 5% of the analytical solution for $\tau > 100$ will be considered acceptable.

4.8 Test of Heat and Mass Transfer in Porous Media

4.8.1 Purpose

In some special instances, the flow of a hot fluid in a confined aquifer may be described by an analytical expression. Avdonin (1964) presents an analytical solution for one-dimensional, radial fluid flow with heat conduction in the orthogonal direction. In addition to testing the coupled heat- and mass-transfer implementation for a single-phase system, the results will also demonstrate that the radial geometry is correctly implemented with different grid spacings.

4.8.2 Functional description

The test suite consists of a set of simulations of 1-D radial flow into a confined aquifer. The same flow problem is run with the domain divided into 84 nodes (41 elements), 400 nodes (199 elements), and 800 nodes (399 elements). In addition to demonstrating that the heat- and mass-transfer problem has been correctly formulated and that the radial geometry has been correctly implemented, this test will assess the impact of finer spatial discretization on accuracy.

4.8.3 Assumptions and limitations

The analytical solution presented by Avdonin (1964) takes the form:

$$u(\omega, \tau) = \frac{1}{\Gamma(v)} \left(\frac{\omega^2}{4\tau} \right)^v \int_0^1 \exp\left(-\frac{\omega^2}{4\tau s}\right) \operatorname{erfc}\left(\frac{\alpha s \sqrt{\tau}}{2\sqrt{1-s}}\right) \frac{ds}{s^{v+1}},$$

$$\text{where } \omega = \frac{2r}{b},$$

$$\tau = \frac{4\kappa_t t}{c_t \rho_t b^2},$$

$$v = \frac{qc_w \rho_w}{4\pi b \kappa_t},$$

$$\alpha = \left(\frac{\kappa_r c_r \rho_r}{\kappa_t c_t \rho_t} \right)^{1/2},$$

erfc is the complimentary error function, Γ is the gamma function, r is the radial coordinate, q is the injection flow rate, u is a dimensionless temperature change, and the integration variable s represents a dimensionless time. The subscripts r , w , and t refer to rock, water, and total (rock and water), respectively. The temperature is computed using:

$$T = T_0 - u(\omega, \tau) \cdot (T_0 - T_{in}).$$

This problem assumes one-dimensional, radial, steady-state flow and unsteady heat transport in a single-phase liquid. It simulates the injection

of cool water into a geothermal reservoir. Figure 9 shows the problem geometry with boundary and initial conditions. Input parameters defining the problem are given in Table 28.

Figure 9. Schematic diagram of the Avdonin problem geometry with boundary and initial conditions.

4.8.4 Summary of test cases

4.8.4.1 Heat and mass transfer in a 1-D radial aquifer

4.8.4.1.1 Function Tested. This test verifies that FEHM correctly models 1-dimensional heat and mass transport for radial flow and demonstrates the impact of finer spatial discretization on accuracy.

4.8.4.1.2 Test Scope. This test case is a verification test.

4.8.4.1.3 Requirements Tested. Requirements 3.1, "Finite-Element Coefficient Generation," 3.2, "Formulate Transient Equations" (specifically Sections 3.2.2 and 3.2.6), 3.3, "Apply Constitutive Relationships" (specifically Section 3.3.1), 3.4, "Compute Solution to Transient Equations," and 3.5, "Provide Input/Output Data Files," of Chapter I are verified by this test.

4.8.4.1.4 Required Inputs. Problem input is provided in the following files:

- *avdonin.in*: basic input data used in conjunction with the following geometry data files:
- *avdonin.geom.84*: (84 nodes, 42 elements),
- *avdonin.geom.400*: (400 nodes, 199 elements), or
- *avdonin.geom.800*: (800 nodes, 399 elements).

4.8.4.1.5 Expected Outputs. Values from FEHM, for temperature versus time at a fixed radius ($r = 37.5$ m), and values for temperature versus radius ($r = 0$ to 1000 m) at a specified time, ($t = 1.e9$ s) will be output and compared to the analytical solution. Values within 5% of the analytical solution will be considered acceptable.

Table 28. Input parameters for the Avdonin problem

Parameter	Symbol	Value
Reservoir permeability	k	10^{-12} m^2
Reservoir porosity	ϕ	0.2
Rock thermal conductivity	k_r	$20 \frac{\text{W}}{\text{m} \cdot \text{K}}$
Rock density	ρ_r	2500 kg/m^3
Rock specific heat	C_r	$1000 \frac{\text{J}}{\text{kg} \cdot \text{K}}$
Reservoir thickness	b	200 m
Node spacing (vertical)	Δb	200 m
Reservoir length (radial)	r	0 - 1000 m
Node spacing (radial)	Δr	25 m
84-node domain		0.64 - 12 m
400-node domain		0.32 - 12 m
800-node domain		
Injection rate	q	10 kg/s
Injection temperature	T_{in}	160°C
Initial temperature	T_0	170°C
Initial pressure	P_0	5 MPa
Time step	Δt	50 days
Total elapsed time	t	$1 \cdot 10^9 \text{ s}$
Boundary conditions:		
At $r = r_w = 0 \text{ m}$,	$T(t) = 160^\circ\text{C}, q = 10 \text{ kg/s}$	
At $r = 1000 \text{ m}$,	$T(t) = 170^\circ\text{C}, P(t) = 5 \text{ MPa}$	

4.9 Test of Toronyi Two-phase Problem

4.9.1 Purpose

This problem has evolved into a standard test case for checking two-phase heat and mass transfer (Toronyi and Farouq Ali 1977). Fluid is discharged from a two-phase geothermal reservoir, and the saturation at each node is simulated. There is no analytical solution for this problem; comparisons must be made with other transient heat- and mass-transfer codes. The problem tests the multiphase capabilities severely, and in doing so, verifies that the liquid- and vapor-phase-transport submodels of FEHM are working properly.

4.9.2 Functional description

The test suite consists of a simulation of fluid discharge from a two-phase aquifer. In addition to demonstrating that the heat- and mass-transfer problem has been correctly formulated, it will demonstrate that phase partitioning has been correctly implemented.

4.9.3 Assumptions and limitations

Fluid is discharged at a constant rate from the two-phase geothermal reservoir until 19% of the original water mass has been removed (78.31 days). There is no flow across the peripheral boundaries. Temperature is controlled by the saturation pressure/temperature curve.

The solution is verified by comparison of FEHM results to those found by Thomas and Pierson (1978). Thomas and Pierson used cell-centered elements, whereas FEHM uses node-centered elements, so boundary elements were adjusted to provide matching central nodes. The reservoir model (solution domain) is shown in Fig. 10 along with the node saturations obtained by Thomas and Pierson. The asymmetry in the solution is due to the off-center location of the discharge node. Table 29 lists the input parameters for the Toronyi problem.

4.9.4 Summary of test cases

4.9.4.1 Toronyi two-phase problem

4.9.4.1.1 Function Tested. This test verifies that FEHM has correctly implemented heat and mass transfer and phase partitioning.

4.9.4.1.2 Test Scope. This test case is a verification test.

4.9.4.1.3 Requirements Tested. Requirements 3.1, "Finite-Element Coefficient Generation," 3.2, "Formulate Transient Equations" (specifically Sections 3.2.2 and 3.2.6), 3.3, "Apply Constitutive Relationships" (specifically Section 3.3.1), 3.4, "Compute Solution to Transient Equations," and 3.5, "Provide Input/Output Data Files," of Chapter I are verified by this test.

Figure 10. Solution domain and saturation results for the Toronyi problem.

4.9.4.1.4 Required Inputs. Problem input is provided in the following file:

- *toronyi.in*: basic input and geometry data (64 nodes, 49 elements).

4.9.4.1.5 Expected Outputs. Values from FEHM, for saturation at each interior node at time $t = 78.31$ days, will be output and compared to the Thomas and Pierson (1978) saturation data. Values within 5% of the Thomas and Pierson solution will be considered acceptable.

Table 29. Input parameters for the Toronyi two-phase problem

Parameter	Symbol	Value
Reservoir permeability	k	$9.869 \times 10^{-13} \text{ m}^2$
Reservoir porosity	ϕ	0.05
Rock thermal conductivity	κ_r	$1.73 \frac{\text{W}}{\text{m} \cdot \text{K}}$
Rock density	ρ_r	2500 kg/m^3
Rock specific heat	C_r	$1000 \frac{\text{J}}{\text{kg} \cdot \text{K}}$
Aquifer length	x	1828 m
Node spacing (x) [‡]	Δx	304.666
Aquifer width	y	182.8 m
Node spacing (y) [‡]	Δy	30.4666
Reference temperature	T	250°C
Initial pressure	P_0	4.3 MPa
Initial water saturation	S_{l0}	0.2
Residual liquid saturation	S_{lr}	0.05
Residual vapor saturation	S_{lv}	0.05
Capillary pressure at zero saturation	P_{capmax}	1.0 MPa
Saturation at which capillary pressure goes to zero	S_{lmax}	1.0
Aquifer discharge	q_m	$0.5 \frac{\text{kg}}{\text{m} \cdot \text{s}}$
Initial pressure	P_0	4.4816 MPa
Time step	Δt	10 days
Total elapsed time	t	78.31 days
Boundary conditions: At $x = 1066.33333$, $y = 106.63333$ $q_m = 0.5 \frac{\text{kg}}{\text{m} \cdot \text{s}}$ No flow across peripheral boundaries		
‡ For the FEHM simulation, node spacing around the periphery is half the general spacing to facilitate comparison with Thomas and Pierson who used cell-centered elements, whereas FEHM uses node-centered elements.		

4.10 Test of DOE Code Comparison Project, Problem Five, Case A

4.10.1 Purpose

This model of a 2-D areal reservoir with multiphase flow was developed as part of the DOE Code Comparison Project (Molloy 1980). The two-phase (water/water vapor), heat- and mass-transfer problem is characterized by a moving two-phase boundary. The modeled region has a cold fluid boundary that provides fluid to the system as discharge occurs through a well. Numerical difficulties can occur as nodes go from two-phase to compressed water. This problem is a good test for the two-phase routines, as well as the phase-change algorithm. In addition, this problem provides a test of the code restart capabilities as the initial temperature field is input through use of a restart file. There is no analytical solution for this problem, but results from other codes (Pritchett 1980) are available as a check for FEHM.

4.10.2 Functional description

The test suite consists of a simulation of fluid discharge from a two-phase, 2-D aquifer. Fluid produced at the production well is replaced by cold-water recharge over the length of one of the lateral boundaries. In addition to demonstrating that the heat- and mass-transfer problem has been correctly formulated, the test suite will demonstrate that phase partitioning has been correctly implemented.

4.10.3 Assumptions and limitations

Fluid is discharged from the two-phase geothermal reservoir whereas cold-water recharge occurs over one lateral boundary. The other three boundaries are considered to be impermeable and nonconductive. The geometry and boundary conditions are shown in Fig. 11. Of particular note is the variable initial-temperature field and the prescribed pressure and temperature boundary. Table 30 lists the input parameters for the DOE Code Comparison Project problem. A Corey-type relative permeability function is used for this model (see Zyvoloski 1997a, "Relative Permeability and Capillary Pressure Functions" in Section 8.4.3). The reader is referred to Pritchett (1980) for a more detailed discussion of this problem and the code comparison. The solution is verified by comparison of FEHM results to other codes (obtained from Pritchett).

4.10.4 Summary of test cases

4.10.4.1 DOE Code Comparison Project, Problem Five

4.10.4.1.1 Function Tested. This test verifies that FEHM has correctly implemented heat and mass transfer and phase partitioning.

4.10.4.1.2 Test Scope. This test case is a verification test.

Figure 11. Schematic diagram of the geometry and boundary conditions for the DOE Code Comparison Project problem.

4.10.4.1.3 Requirements Tested. Requirements 3.1, "Finite-Element Coefficient Generation," 3.2, "Formulate Transient Equations" (specifically Sections 3.2.2 and 3.2.6), 3.3, "Apply Constitutive Relationships" (specifically Section 3.3.1), 3.4, "Compute Solution to Transient Equations," 3.5, "Provide Input/Output Data Files," and 3.6, "Provide Restart Capability" (specifically Sections 3.6.2 and 3.6.3), of Chapter I are verified by this test.

4.10.4.1.4 Required Inputs. Problem input is provided in the following files:

- *doe.dat*: basic input and geometry data (140 nodes, 117 elements) and
- *doe.ini*: initial temperature field, pressure, and saturation.

4.10.4.1.5 Expected Outputs. Values from FEHM for production-well temperature and pressure and pressure at the observation well versus time will be output and compared to the data from other codes. Values within 5% of those obtained by the other codes will be considered acceptable.

Table 30. Input parameters for the DOE Code Comparison Project, Problem 5, Case A

Parameter	Symbol	Value
Reservoir permeability	k	$2.5 \times 10^{-14} \text{ m}^2$
Reservoir porosity	ϕ	0.35
Rock thermal conductivity	κ_r	$1 \frac{\text{W}}{\text{m} \cdot \text{K}}$
Rock density	ρ_r	2563 kg/m^3
Rock specific heat	C_r	$1010 \frac{\text{J}}{\text{kg} \cdot \text{K}}$
Reservoir length	x	300 m
Reservoir thickness	y	200 m
Node spacing [‡]	$\Delta x, \Delta y$	25 m
Liquid residual saturation	S_{lr}	0.3
Gas residual saturation	S_{vr}	0.1
Reservoir discharge	q_m	$0.05 \frac{\text{kg}}{\text{m} \cdot \text{s}}$
Initial pressure	P_0	3.6 MPa
Time step	Δt	30 - 60 days
Total elapsed time	t	10 years
Production-well coordinates: $x = 62.5 \text{ m}, y = 62.5 \text{ m}$ Observation-well coordinates: $x = 162.5 \text{ m}, y = 137.5 \text{ m}$		
Initial temperature distribution: $[T \text{ in } ^\circ\text{C}, r \text{ in m (} r = \sqrt{x^2 + y^2} \text{)}]$: $T(x, y, 0) = \begin{cases} 240 & 0 \leq r \\ 240 - 160\left(\frac{r-100}{200}\right)^2 + 80\left(\frac{r-100}{200}\right)^4 & 100 < r < 300 \\ 160 & r \geq 300 \end{cases}$		
Boundary conditions: At $x = 62.5 \text{ m}, y = 62.5 \text{ m}$ $q_m = 0.5 \frac{\text{kg}}{\text{m} \cdot \text{s}}$ At $x = 300 \text{ m}, y = 0 - 200 \text{ m}$ $T = 160^\circ\text{C}, P = P_0 = 3.6 \text{ MPa}$ At $x = 0 \text{ m}, y = 0 \text{ m}, y = 200 \text{ m}$ Impermeable, nonconductive		
[‡] For the FEHM simulation, node spacing around the periphery is half the general spacing (12.5 m).		

4.11 Test of Dry-out of a Partially Saturated Medium

4.11.1 Purpose

Calculations of fluid flow in the presence of repository heat require the simultaneous solution of a heat- and mass-transfer system consisting of water, water vapor, and air. This test case exercises the code option that solves this type of flow and heat-transport problem by passing air through a one-dimensional, partially saturated medium. The air evaporates water and removes it from the system. A dry-out zone progresses from the injection region through the flow path at a rate that can be predicted using an analytical solution.

4.11.2 Functional description

The test suite consists of a simulation of the rate of movement of a dry region, starting at a condition of constant saturation throughout the flow path. Two cases are considered: a system without vapor-pressure lowering and one with vapor-pressure lowering, which lowers the water-vapor carrying capacity of the injected air.

4.11.3 Assumptions and limitations

If dry air is injected into a partially saturated medium containing immobile liquid water, the water evaporates until the partial pressure of water vapor in the gas reaches its equilibrium vapor pressure. For a mass flow rate of air of $\dot{m}_a$ and assuming ideal-gas-mixture conditions, the corresponding rate of removal of water in the gas $\dot{m}_w$ is given by

$$\dot{m}_w = \frac{M_w P_w \dot{m}_a}{M_a P_a},$$

where M_w and M_a are molecular weights and P_w and P_a are partial pressures with the subscripts w and a referring to the water and air, respectively. Assuming that the dry-out occurs as a sharp front, the rate of progression of this front can be shown to be

$$r_{dry} = \frac{L \dot{m}_a M_w P_w}{\phi S V \rho_w M_a P_a}.$$

In this equation, L is the flow path length, V is the volume, and S is the liquid saturation. The problem is depicted in Fig. 12. Table 31 lists the input parameters used in this comparison. When vapor-pressure lowering is included, the value of P_w in the equation is lower than it would be in the absence of this effect. The capillary pressure in these simulations is adjusted so that it is a constant value throughout the column, regardless of saturation. Its value is set using the linear capillary-pressure model such that the water vapor pressure is lowered by a factor of 2.

Figure 12. Schematic drawing of the geometry and boundary conditions for the dry-out simulations.

Table 31. Input parameters for the dry-out simulations		
Parameter	Symbol	Value
Air flow rate	q	$1.0 \cdot 10^{-6}$ kg/s
Volume of path	V	1 m^3
Length of path	L	1 m
Node spacing	Δl	0.005 m
Porosity	ϕ	0.05
Time step	Δt	w/o vapor-pressure lowering $0.001 - 1.5 \text{ days}$
with vapor-pressure lowering		$0.001 - 3 \text{ days}$
Total elapsed time	t	w/o vapor-pressure lowering 500 days
with vapor-pressure lowering		1000 days
Total system pressure	P_0	0.1 MPa
Temperature (from which P_w is computed)	T	20°C
Initial water saturation	S_{l0}	0.2
Residual liquid saturation	S_{lr}	0.3
Residual vapor saturation	S_{lv}	0.3
Maximum liquid saturation	S_{lmax}	1.0
Maximum vapor saturation	S_{vmax}	1.0
Boundary conditions:		
At $l = 0$		$q = 1 \cdot 10^{-6} \text{ kg/s}$
At $l = 1$		$P = 0.1 \text{ MPa}$

4.11.4 Summary of test cases

4.11.4.1 Dry-out without vapor-pressure lowering

4.11.4.1.1 **Function Tested.** This test verifies that FEHM correctly simulates the dry-out of a partially saturated medium in the absence of vapor-pressure lowering.

4.11.4.1.2 **Test Scope.** This test case is a verification test.

4.11.4.1.3 **Requirements Tested.** Requirements 3.1, "Finite-Element Coefficient Generation," 3.2, "Formulate Transient Equations" (specifically Sections 3.2.3 and 3.2.6), 3.3, "Apply Constitutive Relationships" (specifically Sections 3.3.2 and 3.3.4), 3.4, "Compute Solution to Transient Equations," and 3.5, "Provide Input/Output Data Files," of Chapter I are verified by this test.

4.11.4.1.4 **Required Inputs.** Problem input is provided in the following files:

- *dryout1.in*: basic input data and
- *dryout.geom*: geometry data (the grid consists of 201 x 2 nodes, thus simulating a one-dimensional flow system).

4.11.4.1.5 **Expected Outputs.** Values from FEHM for the position of the dry-out front at five different times should agree with the analytical solution. Position within 5% of the predicted value will be considered acceptable.

4.11.4.2 Dry-out with vapor-pressure lowering

4.11.4.2.1 **Function Tested.** This test verifies that FEHM correctly simulates the dry-out of a partially saturated medium when vapor-pressure lowering is included.

4.11.4.2.2 **Test Scope.** This test case is a verification test.

4.11.4.2.3 **Requirements Tested.** Requirements 3.1, "Finite-Element Coefficient Generation," 3.2, "Formulate Transient Equations" (specifically Sections 3.2.3 and 3.2.6), 3.3, "Apply Constitutive Relationships" (specifically Sections 3.3.2 and 3.3.4), 3.4, "Compute Solution to Transient Equations," and 3.5, "Provide Input/Output Data Files," of Chapter I are verified by this test.

4.11.4.2.4 **Required Inputs.** Problem input is provided in the following files:

- *dryout2.in*: basic input data and
- *dryout.geom*: geometry data (the grid consists of 201 x 2 nodes, thus simulating a one-dimensional flow system).

4.11.4.2.5 **Expected Outputs.** Values from FEHM for the position of the dry-out front at five different times should agree with the analytical solution. Position within 5% of the predicted value will be considered acceptable.

4.12 Test of One-dimensional Reactive-Solute Transport

4.12.1 Purpose

Tracers are used extensively to determine travel times and reservoir volumes. Reactive tracers can be used to infer reservoir properties such as temperature and geochemical composition. Reactive tracers will be used in the C-wells testing at Yucca Mountain. Of course, solute transport capabilities are also used to simulate radionuclide migration. A YMP code, SORBEQ (Robinson 1993), has been developed and validated to model one-dimensional reactive-solute flow and adsorption. FEHM will be compared with SORBEQ on a one-dimensional solute problem with equilibrium sorption. This comparison will verify the species transport in one dimension, and because the codes use different numerical techniques (finite differences versus finite elements), this test suite provides an independent check of both codes.

4.12.2 Functional Description

The test suite consists of a simulation of solute transport for five independent species: a conservative solute and species governed by the linear, Langmuir, Freundlich, and modified Freundlich isotherms.

4.12.3 Assumptions and limitations

The problem is depicted in Fig. 13. Table 32 defines the input parameters used for FEHM and SORBEQ simulations. The adsorption parameters are given in Table 33. A fluid-flow steady state is established by injecting fluid at a fixed flow rate at the inlet and applying a constant-pressure boundary condition at the outlet. The solute transport simulation is executed assuming an initial concentration of zero everywhere in the column and injecting fluid with a concentration of unity at the start of the solute transport phase of the simulation. For each solute, the same dispersivity is assumed (0.033 m, equivalent to a dimensionless Peclet number L/α of 30). The inlet concentration remains at unity for the entire simulation.

Figure 13. Schematic drawing of the geometry and boundary conditions for the 1-D reactive-tracer transport problem.

Table 32. Input parameters for the 1-D reactive-tracer transport problem

Parameter	Symbol	Value
Fluid velocity	v	11.2 m/s
Flow path length	L	1 m
Node spacing	Δl	0.005 m
Dispersivity	α	0.033 m
Porosity	ϕ	0.3
Bulk-rock density	ρ_b	2500 kg/m ³
Time step (tracer)	Δt	0.09 - 0.43 s
Total elapsed time	t	100 s
Pressure	P_0	1.0 MPa
Initial concentration	C_0	0.0
Inlet concentration	C_{in}	1
Boundary conditions: At $l = 0$ $C = 1$ At $l = 1$ $P = 1$ MPa, $\frac{\partial C}{\partial x} = 0$		

Table 33. Adsorption parameters for the reactive-tracer transport problem

Adsorption isotherm	α_1	α_2	β
Conservative	0.0	0.0	1.0
Linear	0.25	0.0	1.0
Langmuir	0.24	1.0	1.0
Freundlich	0.12	0.0	0.8
Modified Freundlich	0.48	1.0	0.8

4.12.4 Summary of test cases

4.12.4.1 Reactive-tracer transport

4.12.4.1.1 **Function Tested.** This test verifies that FEHM has correctly implemented reactive-tracer transport.

4.12.4.1.2 **Test Scope.** This test case is a verification test.

4.12.4.1.3 Requirements Tested. Requirements 3.1, "Finite-Element Coefficient Generation," 3.2, "Formulate Transient Equations" (specifically Sections 3.2.4 and 3.2.6), 3.3, "Apply Constitutive Relationships" (specifically Section 3.3.5), 3.4, "Compute Solution to Transient Equations," and 3.5, "Provide Input/Output Data Files," of Chapter I are verified by this test.

4.12.4.1.4 Required Inputs. Problem input is provided in the following file:

- *sorption.in*: basic input and geometry data (402 nodes, 200 elements). A single simulation is performed that contains five noninteracting solutes with sorption parameters defined in Table 33.

4.12.4.1.5 Expected Outputs. Breakthrough curves (concentration at the outlet node for each species versus time) from FEHM will be output and compared to the SORBEQ solutions. When concentrations are close to zero, percent errors are misleading. Furthermore, considerable concentration errors result from only a small displacement of a breakthrough curve along the time axis because of the steep rise of the concentration-time curve for a typical case. Therefore, concentrations within 0.01 of the SORBEQ solutions and percent errors less than 10% when concentrations are greater than 0.1 will be considered acceptable.

4.13 Test of Henry's Law Species

4.13.1 Purpose

This set of verification runs tests the numerous combinations of effects possible for Henry's Law solutes that may sorb or undergo chemical reaction. Two extremes for the one-dimensional flow field are employed: 1) air moving through a stagnant fluid phase and 2) water moving through a stagnant air phase. The solute will partition into the stagnant fluid, resulting in a decrease in the overall solute transport velocity similar to that observed with equilibrium sorption.

4.13.2 Functional description

The problem set has been divided into three segments. Segment 1 covers air moving through a stagnant fluid phase, and Segment 2 covers water moving through a stagnant air phase. Segment 3 contains problems similar to those of Segments 1 and 2 except that chemical reaction is also included for the Henry's Law species. The approach here is to check the results of a Henry's Law species against tests of a liquid- or vapor-only species under conditions designed to give similar breakthrough times. Table 34 outlines the combinations of chemical phenomena exercised in each problem

Table 34. Combinations of phenomena exercised in the tests of Henry's Law species			
Problem	Mobile phase	Sorption	Reaction
1-1	air	none	none
1-2	air	liquid-rock	none
1-3	air	vapor-rock	none
2-1	water	none	none
2-2	water	liquid-rock	none
2-3	water	vapor-rock	none
3-1	water	none	liquid and vapor
3-2	water	liquid-rock	liquid and vapor
3-3	air	vapor-rock	liquid and vapor

4.13.3 Assumptions and limitations

Problem 1-1: A Henry's Law constant (K_H) was chosen so that at any location half of the species resides in the vapor and half in the liquid. In the simulation, the tracer is exchanged between the flowing vapor and stagnant liquid. Therefore, this solute should behave identically to a linearly sorbing solute (see verification in the previous section,

Section 4.12) with a sorption parameter that yields a velocity of one-half the conservative tracer velocity.

Problem 1-2: A Henry's Law constant of twice that of Problem 1-1, combined with an appropriate liquid-borne solute-rock sorption parameter, results in a partitioning of the solute of one-half vapor, one-fourth liquid, and one-fourth sorbed from liquid to rock. The results should be virtually identical to those of Problem 1-1, showing that the coupling of liquid to solid sorption is implemented properly for a Henry's Law species.

Problem 1-3: This problem is similar to Problem 1-2 except that sorption occurs from the vapor to the rock. The results should be virtually identical to those of Problem 1-1.

Problems 2-1, 2-2, and 2-3: These runs are similar to their counterparts in Segment 1, except that the water phase is moving. The breakthrough curves should agree closely with that obtained for a liquid-only species undergoing sorption.

Problem 3-1: This problem tests a Henry's Law species with no sorption but with chemical reaction taking place in both the vapor and liquid (implemented as two independent chemical reactions). The steady-state concentration exiting the reactor is compared to that of a liquid-only species that reacts at twice the rate. Because the solute remains in the system twice as long for the Henry's Law species, rate constants lower by a factor of two for both the liquid and vapor should yield the same steady-state concentration as the liquid-only species.

Problem 3-2: This problem is an extension of Problem 3-1 that includes sorption from liquid to rock. Chemical reaction is specified as taking place in the liquid, vapor, and sorbed phase, with rate constants selected so that the results should agree with those of Problem 3-1. Two cases are tested: Henry's Law with sorption and liquid-only with sorption.

Problem 3-3: This problem is the same as Problem 3-2 except that the air is the moving phase and sorption is from vapor to rock.

The problem geometry is depicted in Fig. 14. Table 35 defines the input parameters, and the adsorption, Henry's law, and reaction parameters are given in Table 36. The problems are isothermal.

Figure 14. Schematic drawing of the geometry and boundary conditions for the tests of Henry's Law species.

Table 35. Input parameters for the tests of Henry's Law species

Parameter	Symbol	Value
Flow rate (liquid flow rate for mobile-liquid case, air flow rate for mobile-air case)	q	$1.0 \cdot 10^{-4}$ kg/s
Flow path length	L	1 m
Node spacing	Δl	0.005 m
Dispersivity	α	0.033 m
Porosity	ϕ	0.05
Permeability		
Mobile air phase	k	$1 \cdot 10^{-11}$ m ²
Mobile water phase		$1 \cdot 10^{-12}$ m ²
Bulk-rock density	ρ_b	2500 kg/m ³
Time step (tracer)		
Mobile air phase	Δt	0.09 - 0.43 s
Mobile water phase		500 s
Total elapsed time (tracer)		
Mobile air phase	t	864 s
Mobile water phase		6 days
Pressure	P_0	0.1 MPa
Reference pressure	P_{ref}	0.1 MPa
Reference temperature	T_{ref}	20°C
Initial water saturation		
Mobile air phase	S_{I0}	0.2
Mobile water phase		0.5
Residual liquid saturation		
Mobile air phase	S_{lr}	0.3
Mobile water phase		0.0
Residual vapor saturation		
Mobile air phase	S_{lv}	0.3
Mobile water phase		0.6
Maximum liquid saturation		
Mobile air phase	S_{lmax}	1.0
Mobile water phase		0.3
Maximum vapor saturation		
Mobile air phase	S_{vmax}	1.0
Mobile water phase		0.0

Table 35. Input parameters for the tests of Henry's Law species (continued)

Parameter	Symbol	Value
Initial concentration	C_0	0.0
Inlet concentration	C_{in}	1
Boundary conditions:	At $l = 0$ At $l = 1$	$C = 1, q = 1.0 \cdot 10^{-4} \text{ kg/s}$ $q = 1.0 \cdot 10^{-4} \text{ kg/s}$

Table 36. Adsorption, Henry's Law, and reaction parameters for the tests of Henry's Law species

Problem	α_1	α_2	β	K_H	Reaction
1-1 (both phases)	0.0	0.0	1.0	33.64	N/A
1-2				67.24	
vapor phase	0.0	0.0	1.0		N/A
liquid phase	$9.4972 \cdot 10^{-6}$	0.0	1.0		
1-3				67.24	
vapor phase	$3.991 \cdot 10^{-3}$	0.0	1.0		N/A
liquid phase	0.0	0.0	1.0		
2-1 (both phases)	0.0	0.0	1.0	134.0127	N/A
2-2				67.00635	
vapor phase	0.0	0.0	1.0		N/A
liquid phase	$4.989 \cdot 10^{-3}$	0.0	1.0		
2-3				67.00635	
vapor phase	$1.191 \cdot 10^{-5}$	0.0	1.0		N/A
liquid phase	0.0	0.0	1.0		
3-1	0.0	0.0	1.0	134.0127	liquid and vapor
3-2				67.00635	
vapor phase	0.0	0.0	1.0		liquid, vapor, and sorbed
liquid-phase adsorption	$4.989 \cdot 10^{-3}$	0.0	1.0		
3-3				67.24	
vapor phase	0.0	0.0	1.0		liquid, vapor, and sorbed
liquid phase	$9.4972 \cdot 10^{-6}$	0.0	1.0		

4.13.4 Summary of test cases

4.13.4.1 Air movement through stagnant water

4.13.4.1.1 Function Tested. This test verifies that FEHM correctly simulates the transport of a species that partitions between a mobile air phase and immobile water.

4.13.4.1.2 Test Scope. This test case is a verification test.

4.13.4.1.3 Requirements Tested. Requirements 3.1, "Finite-Element Coefficient Generation," 3.2, "Formulate Transient Equations" (specifically Sections 3.2.4 and 3.2.6), 3.3, "Apply Constitutive Relationships" (specifically Section 3.3.5), 3.4, "Compute Solution to Transient Equations," and 3.5, "Provide Input/Output Data Files," of Chapter I are verified by this test.

4.13.4.1.4 Required Inputs. Problem input is provided in the following files:

- *henry1-1.in*: basic input data,
- *henry1-2.in*: basic input data,
- *henry1-3.in*: basic input data, and
- *henry.geom*: geometry data (this two-dimensional grid contains 201 nodes in the flow direction and 2 in the direction perpendicular to flow, making this effectively a one-dimensional simulation).

4.13.4.1.5 Expected Outputs. Values from FEHM for concentration versus time at the outlet node will be output and compared to the FEHM solution for a linearly sorbing solute with a retardation factor of 2. Concentrations within 0.01 of the sorbing-solute solution and percent errors less than 10% when concentrations are greater than 0.1 will be considered acceptable.

4.13.4.2 Water movement through stagnant air

4.13.4.2.1 Function Tested. This test verifies that FEHM correctly simulates the transport of a species that partitions between a mobile water phase and immobile air.

4.13.4.2.2 Test Scope. This test case is a verification test.

4.13.4.2.3 Requirements Tested. Requirements 3.1, "Finite-Element Coefficient Generation," 3.2, "Formulate Transient Equations" (specifically Sections 3.2.4 and 3.2.6), 3.3, "Apply Constitutive Relationships" (specifically Section 3.3.5), 3.4, "Compute Solution to Transient Equations," and 3.5, "Provide Input/Output Data Files," of Chapter I are verified by this test.

4.13.4.2.4 Required Inputs. Problem input is provided in the following files:

- *henry2-1.in*: basic input data,
- *henry2-2.in*: basic input data,

- *henry2-3.in*: basic input data, and
- *henry.geom*: geometry data.

4.13.4.2.5 Expected Outputs. Values from FEHM for concentration versus time at the outlet node will be output and compared to the FEHM solution for a linearly sorbing solute with a retardation factor of 2. Concentrations within 0.01 of the sorbing-solute solution and percent errors less than 10% when concentrations are greater than 0.1 will be considered acceptable.

4.13.4.3 Air/water movement through stagnant water/air with chemical reaction

4.13.4.3.1 Function Tested. This test verifies that FEHM correctly simulates the transport of a species that partitions between a mobile air phase and immobile water and for which the solute also undergoes an irreversible, first-order reaction.

4.13.4.3.2 Test Scope. This test case is a verification test.

4.13.4.3.3 Requirements Tested. Requirements 3.1, "Finite-Element Coefficient Generation," 3.2, "Formulate Transient Equations" (specifically Sections 3.2.4 and 3.2.6), 3.3, "Apply Constitutive Relationships" (specifically Sections 3.3.5 and 3.3.6), 3.4, "Compute Solution to Transient Equations," and 3.5, "Provide Input/Output Data Files," of Chapter I are verified by this test.

4.13.4.3.4 Required Inputs. Problem input is provided in the following files:

- *henry3-1.in*: basic input data,
- *henry3-2.in*: basic input data,
- *henry3-3.in*: basic input data, and
- *henry.geom*: geometry data.

4.13.4.3.5 Expected Outputs. Values from FEHM for concentration versus time at the outlet node will be output and compared to the FEHM solution for the input file *henry3-1.in* (species 1). Concentrations within 0.01 of the sorbing-solute solution and percent errors less than 10% when concentrations are greater than 0.1 will be considered acceptable. For input files *henry3-1.in* (species 2), *henry3-2.in*, and *henry3-3.in*, only the steady-state concentration at the end of the simulation will be compared to that for a one-dimensional, plug flow (constant velocity) system with reaction. Values within 5% of the plug flow solution will be considered acceptable.

4.14 Test of Fracture Transport with Matrix Diffusion

4.14.1 Purpose

Matrix diffusion is an important process in the transport of contaminants in fractured porous media. Under certain limiting conditions, analytical solutions have been developed. The transport module of FEHM with equilibrium sorption can be tested in two dimensions against these analytical solutions to ensure that multidimensional transport problems with sorption are properly formulated.

4.14.2 Functional description

The test suite developed here consists of a two-dimensional grid with a permeability field set up to simulate one-dimensional flow in a fracture (a line of nodes along one edge of the model domain). Fluid in the surrounding matrix is stagnant. Tracers injected with the flowing fluid in the fracture can transport into the matrix via molecular diffusion. Sorption can occur either on the fracture, in the matrix, or both. The results for the breakthrough curve (concentration versus time at the outlet of the fracture) can be compared against analytical solutions to test the ability of the code to simulate solute transport with sorption.

4.14.3 Assumptions and limitations

Tang et al. (1981) present an analytical solution for the case of one-dimensional axial dispersion in the fracture coupled to diffusion into an infinite medium (Eqn. 35 in Tang et al. (1981) revised for a fixed observation point a distance L from the inlet and no radioactive decay):

$$\frac{C}{C_{in}} = \frac{2 \cdot \exp\left(\frac{L}{2\alpha}\right)}{\pi^{1/2}} \int_l^\infty \exp\left[-\xi^2 - \frac{L^2}{4\alpha^2\xi^2}\right] \operatorname{erfc}\left(\frac{R_f L \tau}{4\alpha A \xi^2}\right) d\xi,$$

where ξ is the integration variable, R_f is the retardation factor on the fracture, and τ is the mean residence time of fluid through the column. The lower integration bound l and the lumped parameter A are given by

$$l = \frac{L}{2} \left(\frac{R_f}{\alpha v t} \right)^{1/2}$$

and

$$A = \frac{b R_f}{\phi (R_m D_{mol})^{1/2}}.$$

In the above expressions, v is the fluid velocity, t is time, b is the half-width of the fracture aperture, ϕ is the porosity of the matrix, R_m is the retardation factor in the matrix, and D_{mol} is the molecular diffusion coefficient of the solute. If we select a molecular diffusion coefficient such that the tracer has insufficient time to diffuse to the edge of the model domain on the opposite side of the fracture, then the solution of Tang et al. should be replicated by FEHM. For sorption, the analytical solution is given in terms of retardation factors for the fracture and matrix. In FEHM, the expression used to duplicate a retardation factor for a saturated medium is

$$R_f = 1 + \frac{\rho_b K_d}{\phi \rho_f},$$

where K_d is the sorption distribution coefficient. The problem geometry (symmetric about the fracture) is depicted in Fig. 15. Table 37 gives the sorption parameters and Table 38 lists the input parameters and conditions for this test suite. Separate cases are run with no sorption, sorption in the matrix, and sorption in both the fracture and matrix (flow occurs only in the fracture).

Figure 15. Schematic drawing of the geometry and boundary conditions for the fracture transport problem.

4.14.4 Summary of test cases

4.14.4.1 Transport with matrix diffusion, no sorption

4.14.4.1.1 Function Tested. This test verifies that FEHM correctly simulates the transport system consisting of flow and dispersion in a fracture with diffusion into the rock matrix.

4.14.4.1.2 Test Scope. This test case is a verification test.

4.14.4.1.3 Requirements Tested. Requirements 3.1, "Finite-Element Coefficient Generation," 3.2, "Formulate Transient Equations" (specifically Sections 3.2.4 and 3.2.6), 3.3, "Apply Constitutive Relationships" (specifically Section 3.3.5), 3.4, "Compute Solution to Transient Equations," and 3.5, "Provide Input/Output Data Files," of Chapter I are verified by this test.

Table 37. Adsorption parameters for the fracture transport problem

Test		α_1	α_2	β
Transport with matrix diffusion, no sorption	fracture	0.0	0.0	1.0
	matrix	0.0	0.0	1.0
Transport with matrix diffusion, sorption (linear) in the matrix	fracture	0.0	0.0	1.0
	matrix	$7.4074(10^{-2})$	0.0	1.0
Transport with matrix diffusion, sorption in the fracture and matrix	fracture	8.88889	0.0	1.0
	matrix	$7.4074(10^{-2})$	0.0	1.0

4.14.4.1.4 Required Inputs. Problem input is provided in the following files:

- *tangtest1.in*: basic input data and
- *tangtest.geom*: coordinate and element information. The geometry is represented by a two-dimensional grid of 1590 nodes (53 in the direction of flow and 30 in the matrix). The node spacing in the matrix is small near the fracture where concentration gradients are largest.

4.14.4.1.5 Expected Outputs. Values from FEHM for concentration breakthrough curves will be output and compared to the analytical solution results. A root-mean-square error of the difference between the FEHM and Tang solutions less than or equal to 0.01 for concentrations greater than 0.1 will be considered acceptable.

4.14.4.2 Transport with matrix diffusion, sorption in the matrix

4.14.4.2.1 Function Tested. This test verifies that FEHM correctly simulates the transport system consisting of flow and dispersion in a fracture with diffusion into the rock matrix and with sorption occurring in the matrix.

4.14.4.2.2 Test Scope. This test case is a verification test.

4.14.4.2.3 Requirements Tested. Requirements 3.1, "Finite-Element Coefficient Generation," 3.2, "Formulate Transient Equations" (specifically Sections 3.2.4 and 3.2.6), 3.3, "Apply Constitutive Relationships" (specifically Section 3.3.5), 3.4, "Compute Solution to Transient Equations," and 3.5, "Provide Input/Output Data Files," of Chapter I are verified by this test.

Table 38. Input parameters for the test of the matrix-diffusion problem

Parameter	Symbol	Value
Flow path length (x)	L	5000 m
Node spacing along flow path [‡]	Δx	100 m
Model width	y	5 m
Node spacings	Δy	0.001 - 0.5 m
Fluid density	ρ_f	1000 kg/m ³
Bulk-rock density	ρ_b	2700 kg/m ³
Matrix porosity	ϕ	0.05
Pore-water velocity	v	1.5844×10^{-7} m/s
Dispersivity in fracture	α	500 m
Matrix diffusion coefficient	D_{mol}	1.5×10^{-12} m ² /s
Fracture retardation factor	R_f	1 or 25
Matrix retardation factor	R_m	1 or 5
Time step (tracer)	Δt	0.001 - 5000 days
Total elapsed time	t	1500 years
Pressure	P_0	1.0 MPa
Initial concentration	C_0	0.0
Inlet concentration	C_{in}	1
Boundary conditions: At $l = 0$ m $q = v\rho_f\phi = 7.922 \times 10^{-6}$ kg/s At $l = 5000$ m $P = 1$ MPa		
[‡] The node spacing at each edge is 1 m to accomodate boundary conditions.		

4.14.4.2.4 Required Inputs. Problem input is provided in the following files:

- *tangtest2.in*: basic input data and
- *tangtest.geom*: coordinate and element information. The geometry is represented by a two-dimensional grid of 1590 nodes (53 in the direction of flow and 30 in the matrix). The

node spacing in the matrix is small near the fracture where concentration gradients are largest.

4.14.4.2.5 Expected Outputs. Values from FEHM for concentration breakthrough curves will be output and compared to the analytical solution results. A root-mean-square error of the difference between the FEHM and Tang solutions less than or equal to 0.01 for concentrations greater than 0.1 will be considered acceptable.

4.14.4.3 Transport with matrix diffusion and with sorption in the fracture and matrix

4.14.4.3.1 Function Tested. This test verifies that FEHM correctly simulates the transport system consisting of flow and dispersion in a fracture with diffusion into the rock matrix and with sorption occurring in the matrix and on the fracture.

4.14.4.3.2 Test Scope. This test case is a verification test.

4.14.4.3.3 Requirements Tested. Requirements 3.1, "Finite-Element Coefficient Generation," 3.2, "Formulate Transient Equations" (specifically Sections 3.2.4 and 3.2.6), 3.3, "Apply Constitutive Relationships" (specifically Section 3.3.5), 3.4, "Compute Solution to Transient Equations," and 3.5, "Provide Input/Output Data Files," of Chapter I are verified by this test.

4.14.4.3.4 Required Inputs. Problem input is provided in the following files:

- *tangtest3.in*: basic input data and
- *tangtest.geom*: coordinate and element information. The geometry is represented by a two-dimensional grid of 1590 nodes (53 in the direction of flow and 30 in the matrix). The node spacing in the matrix is small near the fracture where concentration gradients are largest.

4.14.4.3.5 Expected Outputs. Values from FEHM for concentration breakthrough curves will be output and compared to the analytical solution results. A root-mean-square error of the difference between the FEHM and Tang solutions less than or equal to 0.01 for concentrations greater than 0.1 will be considered acceptable.

4.15 Test of the Movement of a Dissolved Mineral Front

4.15.1 Purpose

The ability of FEHM to model precipitation and dissolution reactions allows us to develop more sophisticated models to describe the rock-water interactions at the Yucca Mountain site. The analytical solution for a single, sharp-moving, equilibrium mineral front has been used to verify reactive-transport models in the past (i.e., Engesgaard 1991; Walsh et al. 1984). This analytical solution, which assumes no dispersion, is used to verify that FEHM is accurately predicting the velocity of a dissolved mineral front.

4.15.2 Functional description

A one-dimensional transport simulation of calcite ($\text{CaCO}_3(\text{s})$) dissolution is tested. Profiles of concentration versus reactor length, at selected times, will be compared against the analytical solution.

4.15.3 Assumptions and limitations

The precipitation and dissolution of calcite (a common mineral in many soils) are important processes that play a significant role in controlling the pH and alkalinity of groundwater. The dissolution reaction and the solubility product for this problem are

Thus, the transport system (illustrated in Fig. 16) consists of one equilibrium reaction with three species.

Figure 16. Schematic drawing of the geometry and boundary conditions for the calcite-dissolution problem.

The analytical solution for a single dissolved mineral front (Fig. 17) is given by

$$u_{\text{mineral}} = \frac{u \Delta C_{\text{aq}}}{\Delta C_{\text{aq}} + \frac{\rho_b}{\phi} \Delta C_s},$$

where u is the pore-water velocity, u_{mineral} is the velocity of the mineral front, ρ_b is the bulk-rock density, ϕ is the porosity, ΔC_s is the change in solid concentration across the front, and ΔC_{aq} is the change in aqueous

concentration across the front. A list of relevant input parameters and conditions is given in Table 39.

Figure 17. Aqueous and mineral-front profiles modeled by the analytical solution.

4.15.4 Summary of test cases

4.15.4.1 Calcite dissolution in a one-dimensional system

4.15.4.1.1 Function Tested. This test verifies that FEHM correctly simulates the dissolution of a mineral.

4.15.4.1.2 Test Scope. This test case is a verification test.

4.15.4.1.3 Requirements Tested. Requirements 3.1, "Finite-Element Coefficient Generation," 3.2, "Formulate Transient Equations" (specifically Section 3.2.4), 3.3, "Apply Constitutive Relationships" (specifically Section 3.3.6), 3.4, "Compute Solution to Transient Equations," and 3.5, "Provide Input/Output Data Files," of Chapter I are verified by this test.

4.15.4.1.4 Required Inputs. Problem input is provided in the following files:

- *dissolution.in*: basic input data and
- *dissolution.grid*: coordinate and element information (102 nodes, 50 elements to simulate a one-dimensional flow system).

4.15.4.1.5 Expected Outputs. Values from FEHM for the mean concentration of the mineral front will be compared to the analytical solution. Position within 5% of the predicted value will be considered acceptable.

Table 39. Input parameters for the calcite-dissolution problem		
Parameter	Symbol	Value
Reactor length	L	0.5 m
Node spacing	Δl	0.01 m
Fluid density	ρ_f	1000 kg/m ³
Bulk-rock density	ρ_b	1800 kg/m ³
Porosity	ϕ	0.32
Pore-water velocity [‡]	u	9.37x10 ⁻⁶ m/s
Dispersivity	α	0.0067 m
Time step	Δt	100 s
Total elapsed time	t	2.157 days
Pressure	P_0	1.0 MPa
CaCO ₃ initial concentration	C_{0, CaCO_3}	2.0x10 ⁻⁵ mol/kg-solid
Ca initial concentration	$C_{0, \text{Ca}}$	6.26x10 ⁻⁵ mol/kg-water
CO ₃ initial concentration	C_{0, CO_3}	6.26x10 ⁻⁵ mol/kg-water
Ca inlet concentration	$C_{in, \text{Ca}}$	0
CO ₃ inlet concentration	C_{in, CO_3}	0
Boundary conditions:		
At $l = 0$		$u = 9.37 \times 10^{-6}$ m/s
		$C_{in, \text{Ca}} = 0, C_{in, \text{CO}_3} = 0$
At $l = 1$		$P = 1$ MPa
[‡] Flow rate $q = u \rho_f \phi / 2 \text{ nodes} = 0.0014992$ kg/s		

4.16 Test of Multisolute Transport with Chemical Reaction

4.16.1 Purpose

The coupled transport and chemical reaction of multiple species in solution is an important feature of FEHM that will allow us to incorporate more complex processes into radionuclide transport simulations, as well as to model rock-water interactions at the Yucca Mountain site. The most appropriate way to test this feature of the code is by comparison against a code that was designed specifically for such reactive transport simulations. The code we are using for this purpose is called PDREACT (Valocchi and Pastor 1994), a two-dimensional, isothermal, saturated-zone flow and transport code. This comparison will verify the species transport for a simple, one-dimensional saturated flow field for a complex, multiple-interacting species simulation.

4.16.2 Functional description

The suite of reactions described below are simulated for transport in a one-dimensional flow system. Concentration-versus-time breakthrough curves at the flow path exit and concentration of solid species at the exit versus time will be compared for the two codes.

4.16.3 Assumptions and limitations

The application of this test case is the transport of cobalt (Co) in groundwater. Radioactive cobalt is present in the subsurface at several DOE sites. Although its presence as a divalent cation implies that it should sorb strongly to most soils, its migration rate has been shown to be greater than expected due to complexation with EDTA, a decontaminating agent also found in the subsurface of these sites. Much experimental work has gone into studying the transport of Co as CoEDTA, a much less strongly sorbed species. Figure 18 illustrates the transport problem.

Figure 18. Schematic drawing of the geometry and boundary conditions for the cobalt transport problem.

The chemical reactions and equilibrium or rate constants used to perform this code comparison test are:

and

Thus, the transport system consists of 8 species and six reactions, with reactions specified as either equilibrium or kinetically controlled. $Fe(OH)_3$ is so prevalent in the sand that its concentration is assumed to be constant. In addition, this substance does not act as a true species in either simulation. A list of relevant input parameters and conditions for the code comparison are given in Table 40.

4.16.4 Summary of test cases

4.16.4.1 Cobalt transport in a one-dimensional flow system

4.16.4.1.1 Function Tested. This test verifies that FEHM correctly simulates the reactive transport system consisting of both kinetic and equilibrium reactions and with both immobile and aqueous species.

4.16.4.1.2 Test Scope. This test case is a verification test.

4.16.4.1.3 Requirements Tested. Requirements 3.1, "Finite-Element Coefficient Generation," 3.2, "Formulate Transient Equations" (specifically Sections 3.2.4 and 3.2.6), 3.3, "Apply Constitutive Relationships" (specifically Section 3.3.6), 3.4, "Compute Solution to Transient Equations," and 3.5, "Provide Input/Output Data Files," of Chapter I are verified by this test.

4.16.4.1.4 Required Inputs. Problem input is provided in the following file:

- *multi_solute.in*: basic input data, including the finite-element grid with 202 nodes, 100 elements (51 x 2 nodes to simulate a one-dimensional flow system).

Table 40. Input parameters for test of the reactive transport problem

Parameter	Symbol	Value
Reactor length	L	10 m
Node spacing	Δl	0.1 m
Fluid density	ρ_f	1000 kg/m ³
Bulk-rock density	ρ_b	1500 kg/m ³
Porosity	ϕ	0.4
Pore-water velocity	u	1 m/hr
Dispersivity	α	0.05 m
Time step (tracer)	Δt	0.09 - 360 s
Total elapsed time	t	7.25 days
Pressure	P_0	1.0 MPa
Co inlet concentration	$C_{in, Co}$	3.1623×10^{-5} M
Fe inlet concentration	$C_{in, Fe}$	0 M
EDTA inlet concentration	$C_{in, EDTA}$	3.1623×10^{-5} M
Boundary conditions:	At $l = 0$ At $l = 1$	$u = 1$ m/hr $P = 1$ MPa
‡Flow rate $q = u \rho_f \phi / 2 \text{ nodes} = 0.05556$ kg/s		

4.16.4.1.5 Expected Outputs. Values from FEHM for concentration breakthrough curves of aqueous species and concentration-time history at the outlet node for immobile (solid) species will be output and compared to the PDREACT results. Due to the low inlet concentrations, concentrations within 10% for all values that are greater than 10% of the peak value will be considered acceptable.

4.17 Test of Three-dimensional Radionuclide Transport

4.17.1 Purpose

A comparison will be made with TRACRN (Travis and Birdsell 1988), another YMP code, on a three-dimensional, single-phase liquid problem. The problem simulates the transport of a tracer undergoing radioactive decay and thus is of particular interest to the Yucca Mountain Project. This comparison will verify the species transport in three dimensions. TRACRN has been compared against many known analytical solutions. Although no three-dimensional analytical solutions exist, a match between TRACRN and FEHM will give confidence that both are correct. Because the codes use different numerical techniques, the test provides a check for both codes.

4.17.2 Functional description

The transport system described below consists of one aqueous species undergoing radioactive decay. Concentration-time histories at several locations in the model domain will be used to make the comparison.

4.17.3 Assumptions and limitations

The radionuclide being simulated is Americium (^{243}Am), which has a half-life of 432 years. The model domain, depicted in Figure 19, is a cube (100 m on each side). Infiltration at a rate of 10^{-4} kg/s occurs over a 100 m² region (four nodes) on the top of the box, and outflow is allowed over a 900 m² region (36 nodes) on the bottom. The inlet and outlet nodes are offset from each other in plan view so that flow will travel diagonally through the model domain. There is no flow on the remainder of the boundaries. The simulation is run in two parts. After a steady-state flow field is established, a restart run that solves the transport of the radionuclide is carried out. The ^{243}Am is injected with the inlet fluid at a concentration of 1 M. A conservative tracer is also injected with the inlet fluid as an additional check between the two codes. The problem is isothermal. Table 41 lists the input parameters and conditions for this test suite.

4.17.4 Summary of test cases

4.17.4.1 Decay-chain transport in a three-dimensional system

4.17.4.1.1 Function Tested. This test verifies that FEHM correctly simulates the reactive transport system consisting of a radionuclide decay in a three-dimensional flow system. A conservative tracer is also used to verify the three-dimensional tracer transport. In addition, the restart capabilities of the code are verified.

4.17.4.1.2 Test Scope. This test case is a verification test.

Figure 19. Model domain and flow boundary conditions for test of the radionuclide transport problem.

4.17.4.1.3 Requirements Tested. Requirements 3.1, "Finite-Element Coefficient Generation," 3.2, "Formulate Transient Equations" (specifically Sections 3.2.4 and 3.2.6), 3.3, "Apply Constitutive Relationships" (specifically Section 3.3.5), 3.4, "Compute Solution to Transient Equations," 3.5, "Provide Input/Output Data Files," and 3.6, "Provide Restart Capability," of Chapter I are verified by this test.

4.17.4.1.4 Required Inputs. Problem input is provided in the following files:

- *3d_trac.gen_ini.dat*: basic input data for generating restart and coefficient storage files for the steady-state flow field,
- *3d_trac.grid*: finite-element grid, a structured, three-dimensional grid with 10,648 nodes (22 x 22 x 22) and 9261 elements,
- *3d_trac.dat*: basic input data for transport portion of test run,
- *3d_trac.ini*: steady-state flow initialization file (generated during first portion of test run), and
- *3d_trac.stor*: coefficient storage file (generated during first portion of test run).

4.17.4.1.5 Expected Outputs. Values from FEHM for concentration-time histories at specified nodes will be compared to the TRACRN results. A root-mean-square error between FEHM and TRACRN concentrations less than or equal to 0.05, at concentrations greater than 10% of the peak value, will be considered acceptable.

Table 41. Input parameters and conditions for test of the radionuclide transport problem

Parameter	Symbol	Value
Reservoir dimensions	x, y, z	100 m
Node spacing [‡]	$\Delta x, \Delta y, \Delta z$	5 m
Bulk-rock density	ρ_b	2700 kg/m ³
Porosity	ϕ	0.3
Infiltration rate	q	1.0*10 ⁻⁴ kg/s
Dispersivity	α	5.0 m
Time step (tracer)	Δt	2.74 - 10 years
Total elapsed time (tracer simulation)	t	5000 years
Pressure	P_0	1.0 MPa
Reference pressure	P_{ref}	0.1 MPa
Reference temperature	T_{ref}	20°C
Initial water saturation	S_{I0}	1.0
Residual liquid saturation	S_{lr}	0.277
Maximum liquid saturation	S_{lmax}	1.0
van Genuchten model parameters		
Inverse of air entry pressure	α_G	3.34 m ⁻¹
Power in formula	n	1.982
²⁴³ Am inlet concentration	$C_{in, ^{243}Am}$	1 M
Conservative tracer inlet concentration	$C_{in, Cons}$	1 M
Boundary conditions: At $x = 20 - 30$ m, $q = 1.0 \cdot 10^{-4}$ kg/s $y = 20 - 30$ m, $z = 100$ m At $x = 60 - 90$ m $P = 2$ MPa $y = 60 - 90$ m, $z = 0$ m		
[‡] For the FEHM simulation, node spacing around the periphery is half the general spacing (2.5 m).		

Chapter IV:

Verification and Validation Report

1.0 SCOPE OF VERIFICATION AND VALIDATION ACTIVITIES

The overall verification and validation (V&V) effort for the FEHM application consists of rigorous and complete testing of the model, whenever possible, against known analytical solutions of the same problem. An alternative approach for more complex test cases for which no analytical solution exists is to benchmark the code against the results of other numerical models.

2.0 DESCRIPTION OF ENVIRONMENT

Verification of the FEHM application was performed on the following UNIX platforms: Sun SPARC (SunOS 4.3 and SunOS 5.5), SGI (Irix 5.2 and 5.3), HP (HP-UX A.09.05), and IBM (AIX 2), but FEHM should work on any standard UNIX system.

A series of test scripts have been developed to automate the verification procedure. These scripts are described in more detail in the Appendix "FEHM Verification Scripts" in the FEHM "User's Manual" (Zyvoloski et al. 1997b).

3.0 ADDITIONAL VERIFICATION AND VALIDATION ISSUES

This V&V effort attempts to test each of the major submodels in FEHM against an analytical solution or the results of another flow and transport code. Test cases for heat transfer, isothermal fluid flow, coupled heat and mass transfer, and solute transport are included. For any of these individual runs, there are numerous "minor" options available, such as input/output options, the ability to restart calculations, and the ability to set properties on a node-by-node or zone-by-zone basis that are not included in this report. These options have been extensively debugged, tested, and documented, but in the interest of space and time limitations, they are outside the scope of the formal testing effort.

Model validation is another area that is outside the scope of this report. A large field-testing effort is being undertaken in the Yucca Mountain Project to test the validity of the conceptual models and build confidence in them. However, these studies are scientific studies that are not covered in this document, which focuses only on code verification, the process of determining that the physical models have been properly implemented in the computer code.

4.0 DISCUSSION OF TEST RESULTS

The problems discussed below correspond directly to those described in Section 4.0 of Chapter III, "Verification and Validation Plan."

4.1 Testing of Thermodynamic Functions

4.1.1 Enthalpy

These tests verify that the FEHM enthalpy functions provide accurate values of enthalpy as illustrated in Figure 20. The results, compared numerically to the values used to generate the enthalpy functions (found in files *thermo.steam_table_data.liq* and *thermo.steam_table_data.vap*), are given in Table 42. The maximum absolute error for liquid enthalpy was less than 0.003 MJ/kg, and the percent error was less than 0.2%. The maximum absolute error for vapor enthalpy was 0.0001 MJ/kg, and the percent error was less than 0.004%. These results meet the acceptance criteria for this test suite developed in Chapter III, "Verification and Validation Plan."

Table 42. Results of tests of thermodynamic functions			
V&V test	Maximum error	Maximum % error	RMS error
Enthalpy			
Liquid	0.2100e-02	0.1319	0.1732e-04
Vapor	0.9012e-04	0.3129e-02	0.3128e-05
Density			
Liquid	1.522	0.2482	0.2018e-04
Vapor	0.2550e-01	0.5793e-01	0.6295e-04
Compressibility			
Liquid	0.2160e-02	16.00	0.5182e-02
Vapor	1.287	0.1297	0.4074e-03
Viscosity			
Liquid	0.3224e-05	0.5244	0.9222e-04
Vapor	0.3650e-07	0.1601	0.1687e-03
Saturation pressure and temperature			
Pressure	0.2575e-01	0.3000	0.4687e-03
Temperature	1.100	0.4000	0.5943e-03

4.1.2 Density

These tests verify that the FEHM density functions provide accurate values of density as illustrated in Figure 21. The results, compared numerically to the values used to generate the density functions (found in files *thermo.steam_table_data.liq* and *thermo.steam_table_data.vap*), are given in Table 42. The maximum absolute error for liquid density was less than 1.6 m³/kg, and the percent error was less than 0.3%. The maximum absolute error for vapor density was 0.026 m³/kg, and the percent error was less than 0.06%. These results meet the acceptance criteria for this test suite developed in Chapter III.

Figure 20. Comparison of FEHM enthalpies to the *NBS/NRC Steam Tables* data.

Figure 21. Comparison of FEHM densities to the *NBS/NRC Steam Tables* data.

4.1.3 Compressibility (derivative of density with respect to pressure)

These tests verify that the FEHM compressibility functions provide accurate values of compressibility as illustrated in Figure 22. The results, compared numerically to the values used to generate the compressibility

functions (found in files *thermo.compress_data.liq* and *thermo.compress_data.vap*), are given in Table 42. The maximum absolute error for liquid compressibility was less than 0.0022 MPa^{-1} , and the percent error was less than 16%. The maximum absolute error for vapor compressibility was 1.3 MPa^{-1} , and the percent error was less than 0.2%. These results for vapor compressibility meet the acceptance criteria for this test suite developed in Chapter III. The liquid compressibility had a maximum error greater than the acceptance criteria but the root-mean-square (RMS) error was within acceptable limits. Although the absolute maximum error of liquid compressibility is outside the acceptance criteria, it is important to note that this calculated value of liquid compressibility is never used in the governing equations. This fact is shown best in the accurate solution of the fully saturated Theis problem (see Section 4.4), which would be most sensitive to liquid-compressibility deviations.

Figure 22. Comparison of FEHM compressibilities to the NBS/NRC Steam Tables data.

4.1.4 Viscosity

These tests verify that the FEHM viscosity functions provide accurate values of viscosity as illustrated in Figure 23. The results, compared numerically to the values used to generate the enthalpy functions (found in files *thermo.steam_table_data.liq* and *thermo.steam_table_data.vap*), are given in Table 42. The maximum absolute error for liquid viscosity was less than $3.2\text{e-}6 \text{ Pa}\cdot\text{s}$, and the percent error was less than 0.6%. The

maximum absolute error for vapor viscosity was 3.65×10^{-8} Pa·s, and the percent error was less than 0.2%. These results meet the acceptance criteria for this test suite developed in Chapter III.

Figure 23. Comparison of FEHM viscosities to the *NBS/NRC Steam Tables* data.

4.1.5 Saturation pressure and temperature

These tests verify that the FEHM saturation functions provide accurate values of pressure and temperature as illustrated in Figure 24. The results, compared numerically to the values used to generate the saturation functions (found in file *thermo.saturation_data*), are given in Table 42. The maximum absolute error for saturation pressure was less than 0.03 MPa, and the percent error was less than 0.3%. The maximum absolute error for saturation temperature was 1.1°C, and the percent error was less than 0.4%. These results meet the acceptance criteria for this test suite developed in Chapter III.

Figure 24. Comparison of FEHM saturation pressures and temperatures to the *NBS/NRC Steam Tables* data.

4.2 Test of Heat Conduction

4.2.1 2-D heat conduction in a square

These tests verify that FEHM correctly models 2-dimensional heat conduction. They also verify that the finite-element representation of 2-D 3-node triangles (triangular-element meshes), 4-node quadrilaterals (rectangular-element meshes), mixed-element meshes (containing both triangular and rectangular elements), and refined-element meshes (containing rectangular and trapezoidal elements) have been correctly implemented. Figures 25 and 26 show that FEHM results are in good agreement with the analytical solution for the 2-D heat-conduction simulations. The results, compared numerically to the analytical solution (found in files *heat2dout.analyt_pos* and *heat2dout.analyt_time*), are given in Table 43. The maximum absolute error for these four runs was less than 0.9°C, and the percent errors were less than 0.5%. These results meet the acceptance criteria for this test suite developed in Chapter III.

Table 43. Results of the test of 2-D heat conduction			
V&V test	Maximum error	Maximum % error	RMS error
Temperature versus time at $x = y = 0.0$ m			
3-node triangles	0.5808	0.4166	0.7660e-04
4-node quadrilaterals	0.7141	0.3665	0.4060e-04
mixed elements	0.5526	0.2812	0.5129e-04
refined elements	0.8344	0.4315	0.4253e-04
Temperature versus position at $t = 2.16e4$ seconds			
3-node triangles	0.5980	0.3421	0.7418e-03
4-node quadrilaterals	0.7070	0.3651	0.8163e-03
mixed elements	0.6670	0.3466	0.7643e-03
refined elements	0.8615	0.4452	0.8726e-03

4.2.2 3-D heat conduction in a cube

These tests verify that FEHM correctly models 3-dimensional heat conduction. They also verify that the finite-element representation of 3-D 6-node triangular prisms (prism elements), 8-node quadrilateral polyhedrons (brick elements), 4-node tetrahedrals, mixed-element meshes (containing both triangular prisms and quadrilateral polyhedrons), refined-element meshes (containing quadrilateral polyhedrons and trapezoidal polyhedrons), and the finite-volume option have been correctly implemented. Figures 27 and 28 show that FEHM results are in good agreement with the analytical solution for the 3-D heat-conduction simulations. The results, compared numerically to the analytical solution (found in files *heat3dout.analyt_pos* and *heat3dout.analyt_time*), are given in Table 44. The maximum absolute error for these seven runs was less than 1.3°C, and the percent errors were less than 0.7%. These results meet the acceptance criteria for this test suite developed in Chapter III.

Figure 25. Comparison of FEHM and analytical solutions for 2-D heat conduction at coordinate position $x = y = 0$ m.

Figure 26. Comparison of FEHM and analytical solutions for 2-D heat conduction at time $t = 2.16 \times 10^4$ seconds.

Figure 27. Comparison of FEHM and analytical solutions for 3-D heat conduction at coordinate position $x = y = z = 0$ m.

Figure 28. Comparison of FEHM and analytical solutions for 3-D heat conduction at time $t = 2.16 \times 10^4$ seconds.

Table 44. Results of the test of 3-D heat conduction			
V&V test	Maximum error	Maximum % error	RMS error
Temperature versus time at $x = y = z = 0.0$ m			
6-node triangular prisms	0.7855	0.5670	0.1164e-03
8-node quadrilateral polyhedrons	1.018	0.5273	0.6811e-04
4-node tetrahedral mixed elements	1.245	0.6523	0.7690e-04
refined elements	0.8470	0.4347	0.7936e-04
8-node quadrilateral polyhedrons with finite-volume option	1.267	0.6634	0.7874e-04
refined elements with finite-volume option	1.018	0.5273	0.6811e-04
	1.031	0.5341	0.6892e-04
Temperature versus position at $t = 2.16e4$ seconds			
6-node triangular prisms	0.7960	0.5284	0.1056e-02
8-node quadrilateral polyhedrons	0.9910	0.5199	0.1065e-02
4-node tetrahedral mixed elements	1.243	0.6521	0.1158e-02
refined elements	0.8210	0.4402	0.9981e-03
8-node quadrilateral polyhedrons with finite-volume option	1.265	0.6636	0.1124e-02
refined elements with finite-volume option	0.9910	0.5199	0.1065e-02
	1.005	0.5272	0.1076e-02

4.3 Test of Temperature in a Wellbore

This test verifies that FEHM has correctly implemented the heat- and mass-transfer problem and 2-D radial geometry. Figures 29 and 30 show that FEHM results are in good agreement with the analytical solution. The results, compared numerically to the analytical solution (found in files *rameyout.analyt_pos* and *rameyout.analyt_time*), are given in Table 45. The maximum absolute error for this run was less than 1.4°C, and the percent errors were less than 3%. These results meet the acceptance criteria for this test suite developed Chapter III.

Table 45. Results of the temperature in a wellbore test			
V&V test	Maximum error	Maximum % error	RMS error
Temperature versus time			
d = 0 m	0.2570e-01	0.1285	0.3110e-04
d = 1000 m	1.345	2.815	0.1556e-02
d = 2000 m	1.057	1.358	0.1061e-02
Temperature versus depth			
t = 25 days	0.6971	1.026	0.5203e-03

Figure 29. Comparison of FEHM and Ramey analytical solutions for temperature versus time at d = 1000 m and d = 2000 m.

Figure 30. Comparison of FEHM and Ramey analytical solutions for temperature versus depth at $t = 25$ days.

4.4 Test of Pressure Transient Analysis

This test verifies that FEHM has correctly implemented the pressure equations, i.e., the conservation of mass with Darcy's law, and that radial geometry has been correctly implemented. Figures 31 and 32 show that the FEHM results are in good agreement with the analytical solution. The results, compared numerically to the analytical solution (found in files *theisout.analyt_pos* and *theisout.analyt_time*) are given in Table 46. The maximum absolute error for this simulation was less than 0.0003 MPa, and the percent errors were less than 0.03%. These results meet the acceptance criteria for this test suite developed in Chapter III.

Table 46. Results of the test of the pressure transient analysis			
V&V test	Maximum error	Maximum % error	RMS error
Pressure versus time			
at $r = 0.00144$ m	0.1594e-04	0.1593e-02	0.6169e-06
at $r = 3.44825$ m	0.1548e-04	0.1548e-02	0.5902e-06
Pressure versus position			
at $t = 1$ day	0.1564e-04	0.1564e-02	0.1439e-05

Figure 31. Comparison of FEHM and Theis solutions for pressure versus time at $r = 0.00144$ m and $r = 3.44825$ m from the wellbore.

Figure 32. Comparison of FEHM and Theis solutions for pressure versus position at $t = 1$ day.

4.5 Test of Infiltration into a One-dimensional, Layered, Unsaturated Medium

This test verifies that FEHM has correctly simulated the saturation profile for the infiltration into a one-dimensional, layered, unsaturated medium. Figures 33, 34, and 35 show that the FEHM results are in good agreement with the TOUGH2 simulations. Please note that the expanded saturation scale in Fig. 35 exaggerates differences in fracture saturation at low elevations. The results for the equivalent-continuum model (ECM) and double-porosity/double-permeability model (DKM), compared numerically to results from TOUGH2 (found in files *infiltration.tough2.ecm*, *infiltration.tough2.frac*, and *infiltration.tough2.mat*), are shown in Table 47. The RMS error for the equivalent-continuum model simulation was less than 1%, and the maximum percent error was less than 7%. As expected, significant deviations existed at material interfaces for the double-porosity/double-permeability model. These were the result of differences in model formulation for the fracture-matrix interaction terms. It should also be noted that the van Genuchten capillary-pressure functions are singular at $S = 0$, and all codes must use extrapolation techniques to model values approaching 0. Differences in the extrapolation had the greatest effect in the lowest zone where the fracture saturations approach liquid residual values. Although the maximum percent errors for the double-porosity/double-permeability model were large, the RMS errors for this simulation were less than 4%. These results meet the acceptance criteria for this test suite developed in Chapter III.

Table 47. Results of the test of infiltration into a one-dimensional, layered, unsaturated medium

V&V test	Maximum error	Maximum % error	RMS error
Saturation versus elevation			
ECM	0.5660e-01	6.192	0.1430e-02
DKM - matrix saturation	0.8153e-01	17.13	0.2069e-02
DKM - fracture saturation	0.1022e-01	355.0	0.3679e-01

Figure 33. Comparison of FEHM and TOUGH2 saturations for an equivalent-continuum model.

Figure 34. Comparison of FEHM and TOUGH2 matrix saturation for a double-porosity/double-permeability model.

Figure 35. Comparison of FEHM and TOUGH2 fracture saturation for a double-porosity/double-permeability model.

4.6 Test of Vapor Extraction from an Unsaturated Reservoir

This test verifies that FEHM has correctly implemented steady-state gas flow in a 2-D radial system with an isotropic and an anisotropic permeability model. Figures 36 and 37 show that FEHM results are in good agreement with the analytical solutions (found in files *vapextractout_aniso.analyt* and *vapextractout_iso.analyt*) for the vapor-extraction simulations. The results of the numerical comparison to the analytical solutions are given in Table 48. The maximum absolute error in vapor pressure for the isotropic case was less than 0.002 MPa, and for the anisotropic case, it was less than 0.004 MPa. The maximum percent errors were less than 4%, and the RMS errors were less than 0.01 for both models. These results meet the acceptance criteria for this test suite developed in Chapter III.

Figure 36. Comparison of FEHM steady-state vapor pressure (top) with Shan analytical solution (bottom) for an isotropic reservoir.

Figure 37. Comparison of FEHM steady-state vapor pressure (top) with Shan analytical solution (bottom) for an anisotropic reservoir.

Table 48. Results of the test of vapor extraction from an unsaturated reservoir			
V&V test	Maximum error	Maximum % error	RMS error
Vapor pressures at each node			
Isotropic case	0.1983e-02	2.195	0.8838e-04
Anisotropic case	0.3066e-02	3.311	0.1436e-03

4.7 Test of Dual Porosity

This test verifies that FEHM has correctly implemented the dual-porosity formulation. Figures 38, 39, and 40 show that FEHM results are in good agreement with the analytical solution for the dual-porosity simulations. The differences between the analytical and FEHM solutions can be attributed primarily to the fact that the analytical solution uses a steady-state approximation for the matrix flow (lumped 1 node) whereas FEHM uses a transient approximation (2 node) for the matrix material. The results, compared numerically to the analytical solution (found in files *dual1_out.analyt*, *dual2_out.analyt*, and *dual3_out.analyt*), are given in Table 49. The maximum absolute error for these three runs for nondimensional pressure was less than 0.021, and the percent errors were less than 0.8%. These results meet the acceptance criteria for this test suite developed in Chapter III.

Table 49. Results of the dual-porosity test			
V&V test	Maximum error	Maximum % error	RMS error
Dimensionless pressure versus dimensionless time at $r_w = 0.17528$ m			
Case 1	0.1945e-01	0.3530	0.4143e-03
Case 2	0.2070e-01	0.7086	0.5725e-03
Case 3	0.1931e-01	0.6997	0.5360e-03

Figure 38. Comparison of FEHM and analytical solution for dual-porosity case 1, $\lambda = 0.02546$, $\omega = 0.1000$.

Figure 39. Comparison of FEHM and analytical solution for dual-porosity case 2, $\lambda = 25.46$, $\omega = 0.01099$.

Figure 40. Comparison of FEHM and analytical solution for dual-porosity case 3, $\lambda = 164.7$, $\omega = 0.001013$.

4.8 Test of Heat and Mass Transfer in Porous Media

This test suite verifies that the heat- and mass-transfer problem has been correctly formulated, that radial geometry has been correctly implemented and that finer meshes can improve accuracy. Figures 41 and 42 show that FEHM results are in good agreement with the analytical solution. For the 84-node test grid, mesh-discretization errors are apparent. Other differences are probably due to slight differences in the calculation of thermodynamic properties (the analytical solution uses constant properties). The results, compared numerically to the analytical solution (found in files *avdoninout.analyt_pos* and *avdoninout.analyt_time*) are given in Table 50. The maximum absolute error for these three runs was less than 1.3°C, and the percent errors were less than 0.8%. These results meet the acceptance criteria for this test suite developed in Chapter III.

Table 50. Results of the test of heat and mass transfer in porous media

V&V test	Maximum error	Maximum % error	RMS error
Temperature versus time at $r = 37.5$ m			
84-node grid	1.262	0.7776	0.2169e-03
400-node grid	0.4060	0.2487	0.6973e-04
800-node grid	0.3899	0.2384	0.6742e-04
Temperature versus position at $t = 1.e9$ seconds			
84-node grid	0.5230	0.3237	0.1745e-03
400-node grid	0.2815	0.1744	0.3416e-04
800-node grid	0.2815	0.1744	0.2213e-04

Figure 41. Comparison of FEHM and Avdonin analytical solutions for temperature versus time at $r = 37.5$ m from injection well.

Figure 42. Comparison of FEHM and Avdonin analytical solutions for temperature versus position at $t = 1.e9$ seconds.

4.9 Test of Toronyi Two-phase Problem

This test verifies that FEHM has correctly implemented heat and mass transfer and phase partitioning. The results of the numerical comparison to the Thomas and Pierson (1978) solution (found in file *toronyi.saturations*) are given in Table 51. The maximum absolute error in saturation for this run was less than 0.002, and the percent errors were less than 2%. These results meet the acceptance criteria for this test suite developed in Chapter III. Figures 43 and 44 show the Toronyi and FEHM saturation fields for comparison.

Table 51. Results of the test of the Toronyi two-phase problem			
V&V test	Maximum error	Maximum % error	RMS error
Final saturation at each node	0.1542e-02	1.318	0.7718e-03

Figure 43. Toronyi saturation field at $t = 78.31$ days.

Figure 44. FEHM saturation field at $t = 78.31$ days.

4.10 Test of DOE Code Comparison Project, Problem Five, Case A

This test verifies that FEHM has correctly implemented heat and mass transfer and phase partitioning. Figures 45 and 46 show that FEHM results are in good agreement with the other code solutions for the simulation of the DOE Code Comparison Project Problem. The results of the numerical comparison to the other code solutions are given in Table 52. The maximum absolute error in temperature at the production well for this run was less than 2.1°C, the maximum absolute error in pressure at the production well for this run was less than 0.07 MPa, the maximum absolute error in pressure at the observation well for this run was less than 0.04 MPa, and the percent errors were all less than 3%. These results meet the acceptance criteria for this test suite developed in Chapter III.

Table 52. Results of the test of the DOE Code Comparison Project Problem[‡]

V&V test	Maximum error	Maximum % error	RMS error
Temperature at production node			
Code 1	1.356	0.6531	0.7746e-03
Code 2	1.519	0.6469	0.1070e-02
Code 3	1.623	0.6867	0.1259e-02
Code 4	2.003	0.8526	0.1139e-02
Code 5	1.498	0.7299	0.9932e-03
Code 6	1.368	0.5906	0.1379e-02
Pressure at production node			
Code 1	0.5123e-01	1.581	0.1908e-02
Code 2	0.6127e-01	2.022	0.3137e-02
Code 3	0.5347e-01	1.770	0.3235e-02
Code 4	0.6234e-01	2.057	0.3017e-02
Code 5	0.2150e-01	0.7165	0.1199e-02
Code 6	0.2828e-01	0.9396	0.1637e-02
Pressure at observation node			
Code 1	0.2530e-01	0.7312	0.8879e-03
Code 2	0.2534e-01	0.7610	0.7676e-03
Code 3	0.1656e-01	0.4841	0.8250e-03
Code 4	0.2215e-01	0.6652	0.7065e-03
Code 5	0.3449e-01	1.042	0.1879e-02
Code 6	0.3446e-01	1.041	0.2547e-02
[‡] Modelers Code 1 - Geotrans, Inc. Code 2 - Intercomp Code 3 - Lawrence Berkeley Laboratory (LBL) Code 4 - Systems, Science and Software (S-Cubed) Code 5 - Stanford University Code 6 - University of Auckland, New Zealand

Figure 45. Comparison of FEHM production-well temperatures with results from other codes.

Figure 46. Comparison of FEHM production- and observation-well pressure drops with results from other codes.

4.11 Test of Dry-out of a Partially Saturated Medium

This test verifies that FEHM has correctly implemented the heat- and mass-transfer problem that combines water, water vapor, air, and heat transport. Figure 47 shows that the dry-out front computed using FEHM agrees closely with the analytical solution (results found in files *dryout.analyt2-6*) presented in Chapter III for systems with and without vapor-pressure lowering. The region of dried-out rock proceeds as a sharp front with little spreading, and the rate of movement predicted by the code agrees well with the analytical solution. The maximum percent errors in the positions of the front (the position at which the saturation is 0.1, or dried to 50% of its initial value of 0.2) are 1.3% for both the vapor-pressure lowering case and the case without vapor-pressure lowering (Table 53). Both of these errors are less than 5%, and thus these results meet the acceptance criteria for this test suite developed in Chapter III.

Table 53. Results of the test of dry-out of a partially saturated medium

V&V test	Maximum error	Maximum % error	RMS error
Dryout front versus time w/o vapor-pressure lowering			
Time 100 days	0.6392e-04	0.2623	0.1311e-02
Time 200 days	0.2675e-03	0.5489	0.2744e-02
Time 300 days	0.6338e-03	0.8669	0.4334e-02
Time 400 days	0.1076e-02	1.104	0.5518e-02
Time 500 days	0.1585e-02	1.301	0.6504e-02
Dryout front versus time with vapor-pressure lowering			
Time 200 days	0.3110e-03	1.276	0.6380e-02
Time 400 days	0.2973e-03	0.6099	0.3050e-02
Time 600 days	0.8632e-04	0.1181	0.5903e-03
Time 800 days	0.2393e-03	0.2454	0.1227e-02
Time 1000 days	0.6580e-03	0.5399	0.2700e-02

Figure 47. Comparison of FEHM and analytical solutions for the position of a dry-out front in a partially saturated medium. Cases with (top) and without (bottom) the effects of vapor-pressure lowering are included.

4.12 Test of Reactive-Tracer Transport

This test verifies that FEHM has correctly implemented reactive-tracer transport. Figures 48 to 52 show that FEHM results are in good agreement with the SORBEQ solutions. The results, compared numerically to the SORBEQ solutions (found in files *sorbeq_out.cons*, *sorbeq_out.fr*, *sorbeq_out.lang*, *sorbeq_out.lin*, and *sorbeq_out.mfr*) are given in Table 54. The maximum absolute error in concentration for the five isotherms was less than 0.0104, and the percent errors were less than 10% when concentrations were greater than 0.1. These results meet the acceptance criteria for this test suite developed in Chapter III.

Table 54. Results of the test of reactive-tracer transport

V&V test	Maximum error	Maximum % error	RMS error
Concentration versus time at the outlet node			
Conservative	0.9809e-02	9.599	0.2936e-03
Linear	0.4474e-02	2.258	0.1798e-03
Langmuir	0.9049e-02	5.486	0.2411e-03
Freundlich	0.6322e-02	6.252	0.2531e-03
Modified Freundlich	0.1040e-01	3.060	0.2269e-03

Figure 48. Comparison of FEHM and SORBEQ outlet concentrations for the conservative tracer.

Figure 49. Comparison of FEHM and SORBEQ outlet concentrations for the linear isotherm.

Figure 50. Comparison of FEHM and SORBEQ outlet concentrations for the Langmuir isotherm.

Figure 51. Comparison of FEHM and SORBEQ outlet concentrations for the Freundlich isotherm.

Figure 52. Comparison of FEHM and SORBEQ outlet concentrations for the modified Freundlich isotherm.

4.13 Test of Henry's Law Species

4.13.1 Air movement through stagnant water

This test verifies that FEHM has correctly implemented Henry's law solutes for air moving through a stagnant fluid phase. Figure 53 shows that FEHM results are in good agreement with the analytical solution. The results, compared numerically to the analytical solution (found in file *henry1_out.analyt*), are given in Table 55. The maximum absolute error for cases 1-1, 1-2, and 1-3 was less than 0.0027, and the percent errors were less than 3% for concentrations greater than 0.1. These results meet the acceptance criteria for this test suite developed in Chapter III.

Table 55. Results of the test of Henry's Law species			
V&V test	Maximum error	Maximum % error	RMS error
Concentration versus time at the outlet node			
1-1	0.2594e-02	1.877	0.2024e-03
1-2	0.2615e-02	2.144	0.2336e-03
1-3	0.2583e-02	2.122	0.2309e-03
2-1	0.3281e-02	6.645	0.3447e-03
2-2	0.2837e-02	4.858	0.2306e-03
2-3	0.2910e-02	4.927	0.2358e-03
3-1, species 1	0.8266e-03	7.030	0.1795e-03
Final concentration at the outlet node			
3-1, species 2	0.8190e-03	0.2158	0.2158e-02
3-2, species 1	0.5993e-03	0.1579	0.1579e-02
3-2, species 2	0.3797e-03	0.1000	0.1000e-02
3-3, species 1	0.1727e-03	0.4549e-01	0.3164e-03
3-3, species 2	0.4240e-03	0.1117	0.7845e-03

4.13.2 Water movement through stagnant air

This test verifies that FEHM has correctly implemented Henry's Law solutes for water moving through a stagnant air phase. Figure 54 shows that FEHM results are in good agreement with the analytical solution. The results, compared numerically to the analytical solution (found in file *henry2_out.analyt*), are given in Table 55. The maximum absolute error for cases 2-1, 2-2, and 2-3 was less than 0.0033, and the percent errors were less than 7% when concentrations were greater than 0.1. These results meet the acceptance criteria for this test suite developed in Chapter III.

Figure 53. Comparison of FEHM results with the analytical solution for a mobile air phase.

Figure 54. Comparison of FEHM results with the analytical solution for a mobile water phase.

4.13.3 Air/water movement through stagnant water/air with chemical reaction

This test verifies that FEHM has correctly implemented Henry's Law solutes that may sorb or undergo chemical reaction. Figure 55 shows that FEHM results are in good agreement with the analytical solution, i.e., for case 3-1, species 1, the breakthrough curve appears the same as the analytical solution. The results, compared numerically to the analytical solution (found in file *henry3_out.analyt*), are given in Table 55. The maximum absolute error for case 3-1, species 1, was less than 0.00083, and the percent error was less than 8% when concentrations were greater than 0.1. The maximum absolute error for cases 3-1, 3-2, and 3-3 for the final concentration was less than 0.00082, and the percent errors were less than 0.3%. It should be noted for these cases that the RMS error is essentially a single point average. These results meet the acceptance criteria for this test suite developed in Chapter III.

Figure 55. Comparison of FEHM results with the analytical solution for a mobile water phase with reactions.

4.14 Test of Fracture Transport With Matrix Diffusion

This test verifies that FEHM has correctly implemented the solute transport solution with equilibrium sorption in two dimensions. Figure 56 shows that FEHM's numerical solution is in good agreement with the analytical solution of Tang et al. (1981) for test cases that include matrix diffusion with no sorption, sorption in the matrix, and sorption on the fracture surfaces and in the matrix. The slight discrepancies are probably due to numerical errors associated with insufficiently small grid spacings adjacent to the fracture. This would render the solution inaccurate at early times in the simulation when concentration gradients near the fracture are largest. Nonetheless, the agreement is almost certainly adequate for any analysis that would be made using these model results. The results, compared numerically to the analytical solution (found in files *tang1.analyt*, *tang2.analyt*, and *tang3.analyt*), are given in Table 56. The maximum absolute error for these runs was less than 0.028, and the maximum percent errors ranged from 4.7 to 13.4% for concentration values greater than 0.1. The RMS error ranged from 0.0014 to 0.0022. These results meet the acceptance criteria for this test suite developed in Chapter III.

Table 56. Results of the fracture-transport/matrix-diffusion test			
V&V test	Maximum error	Maximum % error	RMS error
Concentration versus time at the outlet node			
No sorption	0.2810e-01	9.094	0.1412e-02
Matrix sorption	0.1759e-01	13.38	0.2205e-02
Fracture and matrix sorption	0.1707e-01	4.662	0.2108e-02

Figure 56. Comparison of FEHM and Tang analytical solutions for concentration versus time for the matrix-diffusion model.

4.15 Test of the Movement of a Dissolved Mineral Front

This test verifies that FEHM has correctly implemented the reactive transport system consisting of one-dimensional transport with the movement of a dissolved mineral front. Figure 57 compares the front location and shape simulated using FEHM to that predicted from the analytical solution. The results agree closely, with FEHM's numerical results exhibiting a very slight spreading of the dissolution front. Nonetheless, the position of the front agrees with the predicted value (found in files *dissolution.analyt2*, *dissolution.analyt3*, and *dissolution.analyt4*) to within a maximum error of 3.9%. This error is less than 5%, and these results meet the acceptance criteria for this test suite developed in Chapter III. It should be noted for this problem that the RMS error is a single point average for each time.

Table 57. Results of a test of the movement of a dissolved mineral front

V&V test	Maximum error	Maximum % error	RMS error
Dissolution front versus time			
Time 20000. s	0.2606e-02	3.889	0.3889e-01
Time 60000. s	0.3516e-02	1.749	0.1749e-01
Time 100000. s	0.7230e-03	0.2158	0.2158e-02

Figure 57. Comparison of FEHM and the analytical solution for the position of the dissolved mineral front at the final time of the simulation.

4.16 Test of Multisolute Transport with Chemical Reaction

This test verifies that FEHM has correctly implemented the transport of multiple, chemically interacting species in solution for a mixed kinetic and equilibrium reaction system. Figure 58 compares the breakthrough curves for aqueous species for FEHM and PDREACT, the code used for the comparison. Figure 59 compares the solid concentrations versus time at the outlet of the system for the two codes. There is excellent agreement between the two codes for this reactive-transport problem. The PDREACT output is found in files *multi.pdreact_CoEDTA_aq.out*, *multi.pdreact_CoEDTA_s.out*, *multi.pdreact_Co_aq.out*, *multi.pdreact_Co_s.out*, *multi.pdreact_EDTA_aq.out*, *multi.pdreact_FeEDTA_aq.out*, *multi.pdreact_FeEDTA_s.out*, and *multi.pdreact_Fe_aq.out*. Table 58 indicates that the percent errors of all species at the outlet were less than 6% for concentrations greater than 10% of their peak values. These results meet the acceptance criteria for this test suite developed in Chapter III. Numerical results for aqueous *EDTA* and *Fe* are not considered because the concentrations are very near zero, and at such low concentrations, a good measure of error is not available.

Table 58. Results of the test of multisolute reactive transport

V&V test	Maximum error	Maximum % error	RMS error
Aqueous-species concentration versus time			
<i>Co</i>	0.4797e-05	1.591	0.9782e-03
<i>CoEDTA</i>	0.1389e-03	3.386	0.2229e-02
<i>FeEDTA</i>	0.4176e-04	2.238	0.1602e-02
Solid-species concentration versus time			
<i>Co</i>	0.2270e-04	1.660	0.9846e-03
<i>CoEDTA</i>	0.7516e-04	5.608	0.3216e-02
<i>FeEDTA</i>	0.2771e-04	3.199	0.2135e-02

Figure 58. Comparison of FEHM and PDREACT for the breakthrough curves of aqueous species.

Figure 59. Comparison of FEHM and PDREACT for the exit concentration versus time for solid species.

4.17 Test of Three-dimensional Radionuclide Transport with Decay Chain

This test verifies that FEHM has correctly implemented the transport module when used to simulate a radionuclide decay-chain transport problem in three dimensions. Figures 60, 61, 62, and 62 compare the concentration-time curves for the radionuclide and conservative tracer that were simulated using both FEHM and TRACRN, the code used for comparison, at four different positions. Regarding the code comparison, the plots indicate that FEHM and TRACRN concentrations agree quite closely at the comparison points. Results from TRACRN are found in files *3d_tracr3d_cons.out* and *3d_tracr3d_am.out*. Considerable concentration errors can result from only a small displacement of a breakthrough curve along the time axis because of the steep rise or fall of the concentration-time curve for a typical case, as seen by the maximum percent errors, which varied from 3 to 15%. However, Table 59 indicates that the RMS errors of all species at each comparison point were less than 0.0042 (or 0.5%) for concentrations greater than 10% of their peak values. These results meet the acceptance criteria for this test suite developed in Chapter III.

Table 59. Results of the test of the three-dimensional decay-chain problem

V&V test	Maximum error	Maximum % error	RMS error
Conservative-tracer concentration versus time			
Point 1	0.5278e-01	6.878	0.1268e-02
Point 2	0.1590e-01	10.98	0.1834e-02
Point 3	0.3643e-02	4.605	0.8533e-03
Point 4	0.1006e-02	2.840	0.1245e-02
²⁴³ Am concentration versus time			
Point 1	0.4776e-01	7.290	0.1468e-02
Point 2	0.1569e-01	15.14	0.3431e-02
Point 3	0.1033e-02	12.77	0.3291e-02
Point 4	0.1965e-04	14.99	0.4166e-02

Figure 60. Comparison of FEHM and TRACRN results for the concentration-time history at position 1.

Figure 61. Comparison of FEHM and TRACRN results for the concentration-time history at position 2.

Figure 62. Comparison of FEHM and TRACRN results for the concentration-time history at position 3.

Figure 63. Comparison of FEHM and TRACRN results for the concentration-time history at position 4.

5.0 CONCLUSIONS AND RECOMMENDATIONS

The computer code FEHM has been subjected to a wide range of comparison tests. The tests have been designed to verify that the underlying equations described in the FEHM document "Summary of Models and Methods" (Zyvoloski et al. 1997a) are correctly and accurately solved. FEHM proved accurate and passed all the criteria tests except one. That test involved liquid compressibility and was discussed in Section 4.1.3 of this chapter. The endeavor has been to be as complete as possible, but there are some capabilities such as particle tracking, air/water diffusion, and use of unstructured grids and some constitutive relationships (such as rock compressibility, variable thermal conductivity, and equation-of-state models) that still need testing. The testing of these features and new capabilities will be covered in future revisions of this document.

Based on the results of the verification runs specified in Chapter III, it is recommended that the FEHM Application be sanctioned for use within the Yucca Mountain Site Characterization Project for problems of the types currently tested.

Appendix A:
Subroutine and Function Calls
within FEHM

Table 1. Subroutine and function calls within FEHMN

Routine	Description	Calls	Called by
main	Program main was added above fehmn so that all arrays would be allocated before being used (required for the IBM).	fehmn	
air_cp	Compute the heat capacity of air and the derivative with respect to temperature.		thrmwc
air_rdof	Reduce the two-degree-of-freedom solution to Richard's equation.	interblock_iso, thrair	airctr, gensl2
airctr	Manage the isothermal air/water calculations.	air_rdof, gensl2, headctr, thermw, thrair, <i>min0</i>	bnsver, input, startup, varchk, wrtout
allocmem	Allocate memory to dynamic variable arrays.	mmgetblk, storage_derivatives	fehmn
angle3	Determine the angles of rotation needed to point the z-axis from mass point 'i' to neighbor 'j'.	<i>sqrt</i>	eullag3
anonp	Categorize elements and call routines to generate finite-element coefficients.	determ, gencof, md_nodes, mmgetblk, mmrelblk, sx_combine, storage_derivatives, zeroi_out, <i>abs, iabs, max0, sqrt</i>	startup
area2d_tri	Calculate the total area of a triangle and the three Voronoi areas along each of the three sides.	<i>sqrt</i>	anonp, gncf3
area_vol_gaz	Calculate the area/distance and volume of a tetrahedral.		gncf3

Table 1. Subroutine and function calls within FEHMN (continued)

Routine	Description	Calls	Called by
avs_io	Produce FEHM output in AVS UCD or binary format.	avs_write_cord, avs_write_struct, c_close, file_prefix, namefile2, write_avs_node_con, write_avs_node_mat, write_avs_node_s, write_avs_node_v, write_avs_ucl_header, write_binary_geo, write_binary_header, write_binary_node_con, write_binary_node_mat, write_binary_node_s, write_binary_node_v	contr
avs_write_cord	Output AVS coordinate information for FEHM.		avs_io
avs_write_struct	Output AVS mesh-connectivity information for FEHM.	elem_type	avs_io
bcon	Manage boundary conditions.	abs	csolve, fehmn, startup
bcrp	Calculate Brooks Corey relative permeabilities and capillary pressures.		rlperm
binghm	Calculate pressure drop for Bingham fluid.	cubic, asin, sin, sqrt	permp
bit	Set specified bit to the input state.	and, iand, ishft	geneq1, geneq2, geneqc
bnswr	Call routines to assemble finite-element equations and solve for the Newton-Raphson equations.	airctr, dpdp, gensl1, gensl3, gensl4, outbnd, varchk, abs	fehmn, steady
c_close	C routine to close AVS binary format output file.	close	avs_io
c_open	C routine to open AVS binary format output file.	creat	namefile2
cappr	Calculate capillary-pressure functions.	initdata, null	thermw, thrair, thrmwc
casson	Calculate equivalent Darcy permeability for a Casson fluid.	cubic, fourth, sqrt	permp

Table 1. Subroutine and function calls within FEHMN (continued)

Routine	Description	Calls	Called by
cell_time	Compute fluid residence time for cell and calculate probability of a particle moving to a neighbor node.		part_track
check_sx	Check volumes and finite-element flow coefficients.	<i>max</i>	datchk
close_files	Close all open files.		termio
cnsver	Call routine to generate tracer transport equations and call tracer equation-of-state routines.	coneql, dualta, gencon, gentdp, react, thermc, zeror_out, <i>abs, max</i>	csolve
cntlin	Read I/O file names from control file, set unit numbers, and open files.	null, setunits	cntlio
cntlio	Manage the opening and closing of files using control file input.	cntlin, writeio	iofile, termio
co2ctr	Provide overall control for an isothermal air/water simulation.	humidity, initdata, psatl, <i>abs, exit</i>	fehmn, input, startup, timcrl, wrtout
coeffc	Change coefficients of polynomial fits of the thermodynamic properties specified.		startup
concadiff	Compute diffusion coefficient based on volumetric water content.		coneql, csolve, rdcon
concen	Provide overall control for a tracer simulation.	contrc, csolve, diskc, diskp, plotc1, part_track, rdcon, wrtcon, wrtptrk	contr, contrj, disk, fehmn, input, startup, wrtout
coneql	Generate the equations of tracer transport.	<i>abs, max, sqrt</i>	cnsver, gentdp
coneqlmdnode	Compute the Jacobian and residual terms of the concentration equation associated with multiply defined node connections.		cnsver, gentdp
contr	Write out data for contour plots at specified times.	avs_io, concen, contrj, veloc, <i>max</i>	fehmn, startup, timcrl
contrc	Write out tracer data for contour plots.		concen
contrj	Write to contour plot tape using PATRAN format.	concen, veloc	contr

Table 1. Subroutine and function calls within FEHMN (continued)

Routine	Description	Calls	Called by
crdpdp	Update solution for double-porosity/double-permeability problem.		dppd
csolve	Organize tracer solution so smaller time steps can be used for the tracer solution than for the flow solution.	bcon, cnsver, node_rxn, plotc1, resetttrc, solstore, tyning, wrtcon, <i>abs</i> , <i>dlog10</i> , <i>exp</i> , <i>max</i> , <i>min</i>	concen
ctdpdp	Update concentrations for double-porosity/double-permeability solution.		dppd
cubic	Solve cubic equation.	<i>abs</i> , <i>sqrt</i>	binghm, casson
data	Initialize scalar variables, zero all arrays, and load thermodynamic coefficients.	zeroi_out, zeror_out	fehmn
datchk	Initial value analysis and data check.	check_sx, min_max, <i>abs</i> , <i>max</i> , <i>min</i>	fehmn
dated	Determine the current date and time.	<i>dateh</i> (cray), <i>idate</i> , <i>itime</i> , <i>mod</i> (hp, sun), <i>fdate_</i> (ibm)	disk, fehmn
daycrl	Compute new time-step size using adjusted time-step multiplier if necessary.	<i>log10</i>	timcrl
determ	Evaluate determinates.		anonp
diagnostics	Print out worst residuals.	<i>abs</i>	fehmn
disk	Read and/or write files for restart purposes.	concen, dated, stress, <i>max</i>	fehmn, startup, timcrl
diskc	Read and/or write restart files for tracer variables.		concen
diskp	Read and/or write restart files for particle-tracking variables.		concen
done_macro	Close optional input file.		input, scanin
dppd	Provide overall control for a dual-porosity/dual-permeability solution.	crdpdp, ctdpdp, gensdp, gensdp3, indpdp, rddpdp, varchk	bnsver, gensdp, gensdp3, input, startup

Table 1. Subroutine and function calls within FEHMN (continued)

Routine	Description	Calls	Called by
dpsdp3	Load dual-porosity/dual-permeability solution into solution matrix for three-degree-of-freedom system (air, water, heat).	max	gensdp3
dpsdpfa	Load dual-porosity/dual-permeability solution into solution matrix for an isothermal air/water simulation.	max	gensdp
dpsdpfh	Load dual-porosity/dual-permeability solution into solution matrix for a heat, water, water vapor simulation.	max	gensdp
dpsdpfa	Load dual-porosity/dual-permeability solution into solution matrix for tracer simulation.	abs, max	gentdp
drill	Regulate simulated drilling rate.	max	welbor
dual	Provide overall control for a dual-porosity solution.	dualex, dualfa, dualfh, dualtx, initdata, varchk, max	fehmn, gencon, gensl1, gensl2, gensl4, input, startup, timcr
dualex	Extract dual-porosity solution from primary-variable solution.		dual
dualfa	Compute the Jacobian and residual terms of the mass-balance equations at each node for a dual-porosity isothermal air/water solution.	varchk, max	dual
dualfh	Compute the Jacobian and residual terms of the heat and mass equations at each node for a dual-porosity solution.	varchk, max	dual
dualta	Compute the Jacobian and residual terms of the concentration equation at each node for a dual-porosity solution.	abs, max	cnsr
dualtx	Back substitute to get tracer solution for dual-porosity nodes.		dual
dvacalc	Evaluate air/water-vapor diffusion coefficients.		thrmwc
elem_type	Determine element type.		avs_write_struc

Table 1. Subroutine and function calls within FEHMN (continued)

Routine	Description	Calls	Called by
elem_type_binary	C routine to determine element type.		write_binary_geo
enthp	Calculate enthalpy at a node as a function of temperature and pressure.		fehmn, steady, welbor
eullag3	Convert between two geometric reference frames: given a point i, a nearest neighbor j, and a vector, rotate the vector from x, y, z space to a, b, c space.	angle3	rotate
explicit	Make the equations explicit.	abs, max, min	gensl2
fehmn	Primary controlling routine for finite-element heat and mass transfer in porous media.	tyiming, dated, iofile, setparams, allocmem, data, infiles, flow_boundary_conditions, startup, datchk, timcrl, user, welbor, enthp, bnsver, resetv, varchk, dual, diagnostics, fimpf, bcon, steady, co2ctr, sice, veloc, concen, wrtout, plot, contr, disk, pest, abs, max, mod	main
file_prefix	Determine prefix of input file name.		avs_io, termin
film	Regulate film coefficient.	htcchg, abs, max, sqrt	welbor
fimpf	Calculate fraction of variables over a given tolerance.	abs	fehmn
flow_boundary_conditions	Provide flow boundary condition including time-dependent and distributed (by volume) sources.	flow_boun, headctr, initdata, mmgetblk, mmreblk, zeroi_out, zeror_out, abs, max	fehmn, input, setparams, timcrl
flow_boun	Read and apply boundary and source conditions.	model_setup, time_adjust, abs	flow_boundary_conditions
fixo	Calculate internode fluxes.	near3, abs, max, sqrt	input, wrtout
fourth	Solve fourth-order equation.	abs, sqrt	casson
fprop	Change fluid properties in wellbore and annulus.		welbor
freef	C routine to free allocated memory.	free	mmreblk

Table 1. Subroutine and function calls within FEHMN (continued)

Routine	Description	Calls	Called by
gencof	Call routines to generate finite-element coefficients, perform the numerical integration of the elements.	gncf2, gncf3, mmgetblk, mmrelblk, zeror_out	anonp
gencon	Call routines to generate tracer equations and call solver to obtain Newton-Raphson equations for tracer variables.	dual, mmgetblk, mmrelblk, rd1dof, solve_new, storage_derivatives, max, min, sqrt	cnsver
gendat	Generate coordinates and element information in simple geometric problems.		incoord
geneq1	Generate equations for Newton-Raphson corrections for water/vapor flow without noncondensable gas.	bit, setbit	gensdp, gensdp3, gensl1
geneq2	Generate equations for Newton-Raphson corrections for isothermal air/water solution.	bit, setbit	gensdp, gensl2
geneq3	Generate equations for Newton-Raphson corrections for heat conduction only (i.e., permeability).		gensdp, gensdp3, gensl2, gensl3
geneqc	Generate equations for Newton-Raphson corrections for water and noncondensable gas flow.	bit, psat, setbit, zeolites	gensdp3, gensl4
geneqmdnode	Generate equations to multiply defined nodes.	bit, setbit	mdnodes
gensdp	Solve isothermal air/water equations with full Jacobian (unsymmetrical, 2n by 2n).	dmdp, dmdpfa, dmdpfa, geneq1, geneq2, geneq3, mmgetblk, mmrelblk, nrmiz4, rdof_new, solve_new, storage_derivatives, switch, switchb, abs, max, min, sqrt	dmdp
gensdp3	Solve nonisothermal air/water equations with full Jacobian (unsymmetrical, 3n by 3n).	dmdp, dmdp3, geneq1, geneq3, geneqc, mmgetblk, mmrelblk, normal_dof, rdof_new, solve_new, storage_derivatives, switch, switchb, abs, max, min, sqrt	dmdp

Table 1. Subroutine and function calls within FEHMN (continued)

Routine	Description	Calls	Called by
gensl1	Call routines to generate the Newton-Raphson equations for water-only problems and call equation-solver subroutine to solve the heat- and mass-transfer equations with full Jacobian (unsymmetric, 2n by 2n).	dual, geneq1, mmgetblk, mmrelblk, normal, rdof_new, solve_new, storage_derivatives, switch, switchb, <i>abs, max, min, sqrt</i>	bnsver
gensl2	Call routines to generate the Newton-Raphson equations for isothermal air/water problems and call equation-solver subroutine to solve with full Jacobian.	air_rdof, dual, geneq2, geneq3, airctr explicit, mmgetblk, mmrelblk, normal, rdof_new, solve_new, storage_derivatives, switch, switchb, <i>abs, max, min, sqrt</i>	airctr
gensl3	Call routines to generate the Newton-Raphson equations for heat conduction only and call equation-solver subroutine.	geneq3, mmgetblk, mmrelblk, rd1dof, solve_new, storage_derivatives, <i>abs, max, min, sqrt</i>	bnsver
gensl4	Call routines to generate equations for water/noncondensable-gas problems and call equation-solver subroutine to solve the heat and mass equations with noncondensable gas (full Jacobian, unsymmetric 3n by 3n).	dual, geneqc, mmgetblk, mmrelblk, normal, rdof_new, solve_new, storage_derivatives, switch, switchb, <i>abs, max, min, sqrt</i>	bnsver
gentdp	Solve tracer equations with full Jacobian (unsymmetrical, 2n by 2n).	cone1, dpdpta, mmgetblk, mmrelblk, normal, rdof_new, solve_new, storage_derivatives, thermc, <i>max, min, sqrt</i>	cnsver
getconc	Interpolate between background levels of input concentration for use with the particle tracking.		part_track
geoin	Read element and coordinate information from preprocessor with alternate format.	inmentat, inpatran	incoord
gncf2	Generate 2-D finite-element coefficients.	pebi, shap2r	gencof

Table 1. Subroutine and function calls within FEHMN (continued)

Routine	Description	Calls	Called by
gncf3	Generate 3-D finite-element coefficients.	area_vol_gaz, lubksb0, ludcmp0, pebi3, shap3p, shap3r	gencof
headctr	Manage the head input and change pressures into heads and vice versa.	mmgetblk	airctr, flow_boundary_conditions, input, wrtout
heatb	Modify energy source to account for heat generation at the drill bit.	qhuser, <i>abs</i>	permp, welbor
htcchg	Change the fouling coefficients of drill pipe and casing as function of time and depth.		film
humidity	Calculate the saturation for a given humidity value.	<i>log</i>	co2ctr
incond	Read thermal-conductivity data.	initdata, <i>max</i>	input
incoord	Control reading of input coordinate data.	gendat, geoin, null, <i>iabs</i>	infiles
inctrl	Read control variables.	initdata, <i>abs min0</i>	input
indpdp	Modify fracture volume at nodes for dpdp calculations.		dpdp
infiles	Control reading of input data files.	incoord, input, rang, writeio, zone	fehmn
inflow2	Read flow data input by planes for 3-D models.	null, <i>abs, max0</i>	input
inflow	Read flow data.	initdata, mmgetblk, mmrelblk, <i>abs</i>	input
inhflx	Read heat-flux data.	initdata	input
initdata	Read in an arbitrary number of lines of data and set parameter values at given nodes.	mmgetblk, mmrelblk, null, zeroi_out, <i>abs, nint</i>	co2ctr, dual, flow_boundary_conditions, incond, inctrl, inflow, inhflx, inperm, inpres, inptrk, inrock, inzeol, porosi, rdcon, rddpdp, rdthick, renum, rperm, sice, vcon

Table 1. Subroutine and function calls within FEHMN (continued)

Routine	Description	Calls	Called by
inmentat	Read in geometric data generated by mentat mesh generator.		geoin
innode	Read/find node numbers for output.	near3, null, <i>abs</i>	input
inpatran	Read in geometric data generated by patran mesh generator.		geoin
inperm	Read permeability data.	initdata, <i>max</i>	input
inpres	Read nonuniform pressure and temperature or saturation data.	initdata, mmgetblk, mmrelblk, psat, <i>abs</i>	input
inptrk	Read particle-tracking data.	initdata, null	input
input	Control reading of input data file.	airctr, co2ctr, concen, done_macro, dpdp, dual, flow_boundary_conditions, flxo, headctr, incond, inctrl, inflo2, inflow, inhflx, innode, inperm, inpres, inptrk, inrock, intime, inzeol, md_nodes, null, parse_string, pest, porosi, read_avs_io, read_rxn, renum, rperm, sice, start_macro, sther, stress, thickness, user, varctr, vcon, welbor, zone, <i>abs</i>	infiles
inrock	Read rock-property data.	initdata	input
interblock_iso	Generate interblock flow for air/water equations.		air_rdof
intime	Read time-step input.	null	input
inverf	Calculate the inverse of the error function for a value of x between 0 and 1.	<i>alog10</i>	time_diff
inzeol	Read zeolite-hydration data.	initdata, psat, zeolites, zeror_out	input
iofile	Manage the opening of input and output files.	cntllo, termio	fehm

Table 1. Subroutine and function calls within FEHMN (continued)

Routine	Description	Calls	Called by
lubksb	Perform forward and back substitution for N-degree-of-freedom matrix elements.		node_rxn
lubksb0	Perform forward and back substitution for N-degree-of-freedom matrix elements.		gncf3, normal_dof, pebi3
ludcmp	Perform Gauss elimination on N-degree-of-freedom matrix elements.	<i>abs</i>	node_rxn
ludcmp0	Perform Gauss elimination on N-degree-of-freedom matrix elements.	<i>abs</i>	gncf3, normal_dof, pebi3
mallocf	C routine to allocate memory.	<i>exit, malloc, printf</i>	mmgetblk
md_nodes	Manage multiply defined nodes.	mmgetblk	anonp, input, startup
min_max	Find the minimum and maximum parameter values and their location.		datchk
mmgetblk	Allocate memory to an array.	mallocf	allocmem, anonp, flow_boundary_conditions, gencof, gencon, gensdp, gensdp3, gensl1, gensl2, gensl3, gensl4, gentdp, headctr, inflow, initdata, inpres, md_nodes, pest, set_ptrk, split, startup, storage_derivatives, storsx, thermw, thickness, varctr, zone
mmrelblk	Deallocate array memory.	freef	anonp, flow_boundary_conditions, gencof, gencon, gensdp, gensdp3, gensl1, gensl2, gensl3, gensl4, gentdp, inflow, initdata, inpres, split, startup, thermw, storage_derivatives, storsx, thickness, zone
mod_eqs_ngas	Modify equations if no gas is present.	<i>abs</i>	gensl4

Table 1. Subroutine and function calls within FEHMN (continued)

Routine	Description	Calls	Called by
model_setup	Read in parameters for boundary models.		flow_boun
mult_rxn	Compute the reaction-rate terms for each reaction for the given species and node point.	rxn_product, <i>abs</i> , <i>dlog10</i> , <i>exp</i> , <i>max</i> , <i>min</i>	node_rxn, react
namefile2	Generate name for AVS format output file.	c_open	avs_io
near3	Find nearest node to a set of coordinates (x, y, z).	<i>sqrt</i>	fixo, innode, pest, zone
nearn	Determine the nearest node (n) to a given set of coordinates (x, y).	<i>sqrt</i>	welbor
newton	Calculate pressure drop for Newtonian fluid.	<i>log</i> , <i>log10</i>	permp
node_rxn	Compute the updated concentrations of all species at a given node after constructing an <i>n_{speci} x n_{speci}</i> matrix that includes coupling of the concentrations.	lubksb, ludcmp, mult_rxn	csolve
normal	Normalize Newton-Raphson equations and calculate sum-squared sum of residuals.		gensl1, gensl2, gensl4, gentdp
normal_dof	Normalize equations for coupled problems.	lubksb0, ludcmp0	gensdp3
nrmlz4	Normalize the matrix equations.	<i>abs</i> , <i>max</i>	gensdp
null	Check for null lines or all 0's in lines.	<i>char</i> , <i>len</i>	cntlin, incoord, inflo2, initdata, innode, inptrk, input, intime, rdcon, read_rxn, rlperm, scanin, vcon, zone
outbnd	Test the dependent variables to determine if they are within the bounds set by the thermodynamic properties.		bnsver
parse_string	C routine to parse input line with character, integer, and real input.		input, rdcon, read_rxn
part_track	Control particle-tracking simulation.	cell_time, getconc, ran_sp, set_ptrk, time_diff, time_disp, <i>abs</i> , <i>dbl</i> , <i>exp</i> , <i>max</i> , <i>mod</i> , <i>real</i> , <i>sqrt</i>	concen

Table 1. Subroutine and function calls within FEHMN (continued)

Routine	Description	Calls	Called by
pebi	Calculate internodal area using perpendicular bisectors (2-D).	<i>mod, sqrt</i>	gncf2
pebi3	Calculate internodal volume using perpendicular bisectors (3-D).	ludcmp0, lubksb0, <i>abs</i>	gncf3
peint	Set up initial temperature gradients where gradient information is user specified.	<i>abs, max</i>	startup
permp	Calculate equivalent Darcy permeability for pipe flow.	binghm, cason, heatb, newton, power, <i>abs, max</i>	welbor
pest	Parameter estimation I/O routine.	mmgetblk, near3	fehmn, input
plot	Write out data for time-history plots at particular nodes.		fehmn, startup, timcrl
plotc1	Write out tracer data for time-history plots. Print out at flow time steps.		concen, csolve, rdcon, set_ptrk
porosi	Read in data for pressure-dependent porosity and permeability models and calculate porosity and permeability functions.	initdata, welbor, <i>iabs</i>	input, startup, thermw, thrair, wrtout
power	Calculate equivalent permeability for power-law fluid.	<i>log, log10</i>	permp
psat	Calculate the saturation pressure of water for a given temperature.	<i>abs</i>	geneqc, inpres, inzeol, thermw
psatl	Calculate the saturation temperature or pressure.	vaporl, <i>abs</i>	co2ctr, thrmwc, varchk
qhuser	User-specified dissipation rate.		heatb
radius	Modify finite-element coefficients to obtain a radial model.	<i>min, max</i>	startup
ran_sp	Generate a pseudorandom number with a uniform distribution between 0 and 1.	<i>mod, real</i>	part_track, time_diff
rarng	Rearrange 3-D coordinates to obtain 2-D problems when enabled.		infiles

Table 1. Subroutine and function calls within FEHMN (continued)

Routine	Description	Calls	Called by
rd1dof	Solve the equations generated for heat conduction by a reduced degree-of-freedom method.	solve, <i>sqrt</i>	gencon, gensl3
rdcon	Read in tracer data and initialize tracer variables.	initdata, null, parse_string, plotc1, thermc, userc, <i>abs</i> , <i>dlog10</i> , <i>exit</i> , <i>exp</i> , <i>max</i> , <i>min</i>	concen
rddpdp	Read the input data for a dpdp solution.	initdata	dpdp
rdof_new	Reduce a 3n x 3n matrix into a 2n x 2n matrix or an n x n matrix using the RDOF or IRDOF algorithms.	solve_new	gensdp, gensdp3, gensl1, gensl2, gensl4, gentdp
rdthick	Read input data for variable thickness.	initdata	thickness
react	Compute the reaction terms and add to the Jacobian and the residual for each node.	mult_rxn, <i>abs</i> , <i>max</i>	cnsver
read_avs_io	Read input file and set io flags.		input
read_rxn	Read the data for multiple, interacting solutes.	null, parse_string, setup_rxn, <i>abs</i>	input
read_sx	Read finite-element coefficients.		storsx
renum	Read node-renumbering data.	initdata	input
resettrc	Reduce time step of the solute-transport calculation and reset the values of all parameters before reinitiating the calculation.		csolve
resetv	Reset the dependent variables to the last time step value. Used when iteration limits are exceeded and a particular time step is restarted.		fehmn
rlperm	Calculate relative-permeability functions for vapor and liquid.	bcr1p, null, initdata, vgcap, vgcap_fit, vgr1p, welbor, <i>max</i>	input, thermw, thrair, thrmw
rock	Regulate rock properties.	<i>max0</i>	welbor
rotate	Initiate 3-D matrix rotation.	eullag3	cone1, csolve
rxn_product	Compute the reaction-rate terms for each reaction for the given species and node point.	<i>max</i>	mult_rxn

Table 1. Subroutine and function calls within FEHM (continued)

Routine	Description	Calls	Called by
scanin	Scan input file for parameters needed prior to data input.	done_macro, null, start_macro, max	setparams
set_ptrk	Set up starting nodes and times for particle tracking.	mmgetblk, plotc1, abs, int	part_track
setbit	Set specified bit to the input state.	and, iand, ior, ishft, not, or	geneq1, geneq2, geneqc
setord	Set up the order of solution for the equations at each node.		startup
setparams	Initialize/set parameter values.	flow_boundary_conditions, scanin, max	fehm
setunits	Set file unit numbers.		cntlin, termin
setup_rxn	Set up arrays identifying the location and type of a particular species in a reaction.		read_rxn
setzone	Enter properties using geometric zone description.	sfn2r, sfn3r, abs, max, min, sqrt	zone
sfn2r	Evaluate shape functions for 2-D calculations. (Interpolation routine used by zone .)		setzone
sfn3r	Evaluate shape functions for 3-D calculations. (Interpolation routine used by zone .)		setzone
shap2r	Evaluate 2-D finite-element shape functions at quadrature points.	sqrt	gncf2
shap3p	Evaluate 3-D prism-element shape functions at quadrature points.		gncf3
shap3r	Evaluate 3-D quadrilateral-element shape functions at quadrature points.	sqrt	gncf3
sice	Read in data for simulation with ice present.	initdata, sther	fehm, input, startup, wrtout
solstore	Compute the tracer mass storage and sorption terms of the residuals equations and their derivatives.	abs, dlog10, exp, max	csolve, thermc

Table 1. Subroutine and function calls within FEHM (continued)

Routine	Description	Calls	Called by
solve	Solve the one-degree-of-freedom linear system of equations.	<i>abs, max, sqrt</i>	rd1dof
split	Split rectangles/bricks into triangles/tetrahedrals and average so grid orientation is not present.	mmgetblk, mmrelblk, <i>abs, min</i>	startup
start_macro	Allow input to be read from any file.		input, scanin
startup	Perform miscellaneous startup calculations.	airctr, anonp, bcon, co2ctr, coeff, concn, contr, disk, dpdp, dual, md_nodes, mmgetblk, mmrelblk, peint, plot, porosi, radius, setord, sice, slvesu, split, storsx, steady, thickness, tyming, varchk, welbor, zeror_out, <i>abs, max, max0</i>	fehm
steady	Set up initial pressure distribution when gravity is present (enabled).	bnsver, enthpf, <i>abs</i>	startup
sther	Set thermodynamic parameters when simple thermodynamics are invoked.		input, sice
storage_derivatives	Allocate memory for derivative arrays and initialize values, or deallocate derivative arrays.	mmgetblk, mmrelblk, zeror_out	allocmem, anonp, gencon, genspd, genspd3, gensl1, gensl2, gensl3, gensl4, gentdp
storsx	Manage the storage or retrieval of element coefficients from auxiliary file.	mmgetblk, mmrelblk, read_sx	startup
stress	Blank routine that returns without doing anything (for compatibility with other versions of FEHM).		disk, input, wrtout
switch	Reorder the "a" matrix.		genspd, genspd3, gensl1, gensl2, gensl4
switchb	Reorder the "b" matrix.		genspd, genspd3, gensl1, gensl2, gensl4
sx_combine	Combine dimensions of a variable.		anonp

Table 1. Subroutine and function calls within FEHMN (continued)

Routine	Description	Calls	Called by
termin	Read I/O file names from terminal, set unit numbers, and open files.	file_prefix, setunits	termio
termio	Manage the opening and closing of files using terminal input.	close_files, cntlio, termin, writeio	iofile
thermc	Evaluate tracer equation-of-state information.	solstore, userc, <i>abs</i> , <i>dlog10</i> , <i>exp</i> , <i>max</i>	cnsver, gentdp, rdcon
thermw	Evaluate the thermodynamic properties (density, enthalpy, and viscosity) as a function of pressure and temperature (or saturation).	cappr, mmgetblk, mmrelblk, porosi, psat, rlperm, vfcal, welbor, <i>abs</i>	airctr, varchk
thickness	Modify volumes and finite-element coefficients to account for variable thickness.	mmgetblk, mmrelblk, rdthick	input, startup
thrair	Calculate coefficients and derivatives for isothermal air/water system.	cappr, porosi, rlperm	airctr, air_r dof
thrmwc	Evaluate the thermodynamic properties (density, enthalpy, and viscosity) as a function of pressure, temperature, and partial pressure of noncondensable gas for water/noncondensable-gas problems.	air_cp, cappr, dvacalc, psatl, rlperm, vfcal, <i>max</i>	varchk
time_adjust	Adjust time if necessary for boundary models.		flow_boun
timcrl	Control time-step information and stopping criteria.	co2ctr, contr, daycrl, disk, dual, flow_boundary_conditions, plot, <i>abs</i> , <i>iabs</i>	fehmn
time_diff	Compute diffusion time for a particle.	inverf, ran_sp	part_track
time_disp2	Compute dispersion time for a particle.		part_track
tying	Calculate CPU time for a particular computer run. Call is made to the system clock of the computer on which it is run.	<i>second</i> (cray), <i>secnds</i> (hp), <i>etime_</i> (ibm), <i>dblc</i> , <i>etime</i> (sun)	csolve, fehmn, startup

Table 1. Subroutine and function calls within FEHMN (continued)

Routine	Description	Calls	Called by
user	A user-programmed subroutine that provides for changing common block variables every time step. Disabled (i.e., not certified as part of this baseline) for YMP project.		fehmn, input
userc	User-defined subroutine for changing common variables associated with tracer transport. Disabled (i.e., not certified as part of this baseline) for YMP project.		thermc, rdcon
vaporl	Calculate the vapor-pressure-lowering contribution to saturation pressure.	<i>exp</i>	psatl
varchk	Decide, based on current pressure, temperature, and saturation values, on the current phase state (fully saturated, partially saturated). Call routine THERMW or THRMWC to update thermodynamic properties of density, enthalpy, and viscosity. Add the Newton-Raphson corrections to the dependent variables.	airctr, psatl, thermw, thrmwc, vcon, <i>max</i> , <i>max0</i>	bnsver, dpdp, dual, dualfa, dualfh, fehmn, startup
varctr	Convert equations between pressure enthalpy and pressure temperature.	mmgetblk	input
vcon	Calculate variable thermal conductivity.	initdata, null, <i>sqr</i> t	input, varchk
veloc	Calculate fluid velocities in coordinate directions.	<i>abs</i> , <i>max</i> , <i>sqr</i> t	contr, contrj, fehmn
vfcal	Change porosity and permeability as functions of pressure.	<i>exp</i> , <i>log</i>	thermw, thrmwc
vgcap	Compute the capillary pressure and derivatives for the van Genuchten model.		rlperm
vgcap_fit	Provide linear or cubic fit to capillary pressure data.		rlperm
vgrip	Compute the liquid relative permeability and derivative for the van Genuchten model.		rlperm

Table 1. Subroutine and function calls within FEHMN (continued)

Routine	Description	Calls	Called by
volume_tet_voronoi	Find the volume of a tet-element defined by 4 coordinate nodes.	drill, enthp, film, fprop, heatb, nearn, permp, rock, <i>abs</i> , <i>int</i> , <i>log</i> , <i>min</i>	fehm, input, porosi, rperm, startup, thermw
welbor	Do wellbore input and simulation.	drill, enthp, film, fprop, heatb, nearn, permp, rock, <i>abs</i> , <i>int</i> , <i>log</i> , <i>min</i>	fehmn, input, porosi, rperm, startup, thermw
write_avs_node_con	Output AVS concentration fields from FEHM.	<i>min</i> , <i>max</i>	avs_io
write_avs_node_mat	Output AVS scalar-node information for FEHM mesh materials.	<i>float</i>	avs_io
write_avs_node_s	Output AVS scalar-node information for FEHM.		avs_io
write_avs_node_v	Output AVS vector-node information for FEHM.		avs_io
write_avs_ucd_header	Output AVS UCD header information.		avs_io
write_binary_geo	C routine to write AVS binary-coordinate and mesh-connectivity information for FEHM.	elem_type_binary, <i>lseek</i> , <i>write</i>	avs_io
write_binary_header	C routine to write AVS binary UCD header information.	<i>write</i>	avs_io
write_binary_node_con	C routine to write AVS binary concentration fields from FEHM.	<i>lseek</i> , <i>printf</i> , <i>strcat</i> , <i>write</i>	avs_io
write_binary_node_mat	C routine to write AVS binary scalar-node information for FEHM mesh materials.	<i>lseek</i> , <i>printf</i> , <i>strcat</i> , <i>write</i>	avs_io
write_binary_node_s	C routine to write AVS binary scalar-node information for FEHM.	<i>lseek</i> , <i>printf</i> , <i>strcat</i> , <i>write</i>	avs_io
write_binary_node_v	C routine to write AVS binary vector-node information for FEHM.	<i>lseek</i> , <i>printf</i> , <i>strcat</i> , <i>write</i>	avs_io
writeio	Write assigned file names, unit numbers, and file purpose to specified output unit.		cntlio, infiles, termio
wrtcon	Write output for tracer at specified intervals.	<i>abs</i>	concen, csolve

Table 1. Subroutine and function calls within FEHMN (continued)

Routine	Description	Calls	Called by
wrtout	Write output information at a user-specified interval.	airctr, co2ctr, concen, fixo, headctr, porosi, sice, stress, abs, dfloat, max0	fehmn
wrtprk	Output particle-concentration data.		concen
zeolites	Compute the energy/water-source/sink terms due to a zeolite dehydration reaction.	dlog	geneqc, inzeol
zeroi_out	Initialize integer array to zeros.		anonp, data, flow_boundary_conditions, initdata
zeror_out	Initialize real array to zeros.		data, cnsrwer, flow_boundary_conditions, gencoef, inzeol, startup, storage_derivatives
zone	Divide the input problem space by allowing the user to define zones geometrically and then labeling the nodes as to which zone they belong to. These zones are then used to assign properties to the nodes.	mmgetblk, mmrelblk, near3, null, setzone	infiles, input
The following routines, slvesu and solve_new, are reuse components from the GZSOLVE Application ECD-97:			
slvesu	Set up equation solver by identifying fill-in positions in the Newton-Raphson matrix.	N/A	startup
solve_new	Perform preconditioned conjugate gradient solution of a set of linear, algebraic equations.	N/A	gencon, genspd, gensl1, gensl2, gensl3, gensl4, gentdp

Appendix B:
Tests of the Functional Requirements
and Macro Control Statements of
the FEHM Application

1.0 APPENDIX B DESCRIPTION

This appendix contains two tables. Table 1 lists the functional requirements of the FEHM application and, for each requirement, the section in Chapter I that describes that requirement and the sections in Chapter III that describe how that requirement will be tested. Table 2 lists the FEHM macro control statements used by test problems and, for each control statement, the section in the FEHM User's Manual (Zyvoloski et al. 1997b) that describes that macro control statement and the sections in Chapter III that use the control statement in the testing process.

Table 1. Functional requirements of the FEHM application		
Requirement	Chp. I Section	Tested by (Chp. III section[†])
Finite-element coefficient generation	3.1	4.2, 4.3, 4.4, 4.5, 4.6, 4.7, 4.8, 4.9, 4.10, 4.11, 4.12, 4.13, 4.14, 4.15, 4.16, 4.17
Formulate transient equations	3.2	
Heat-conduction equations	3.2.1	4.2
Heat- and mass-transfer equations	3.2.2	4.3, 4.4, 4.5, 4.7, 4.8, 4.9, 4.10
Noncondensable gas flow equations	3.2.3	4.6, 4.11
Solute-transport equations	3.2.4	4.12, 4.13, 4.14, 4.15, 4.16, 4.17
Particle-tracking module	3.2.5	To be developed
Sources and sinks	3.2.6	4.3, 4.4, 4.5, 4.6, 4.7, 4.8, 4.9, 4.10, 4.11, 4.12, 4.13, 4.14, 4.15, 4.16, 4.17
Apply constitutive relationships	3.3	
Pressure- and temperature-dependent water properties	3.3.1	4.1, 4.3, 4.4, 4.7, 4.8, 4.9, 4.10
Properties of air and air/water-vapor mixtures	3.3.2	4.6, 4.11
Equation-of-state models	3.3.3	To be developed
Relative-permeability and capillary-pressure functions	3.3.4	4.5, 4.6, 4.11
Adsorbing solutes	3.3.5	4.12, 4.13, 4.14
Multiple, interacting solutes	3.3.6	4.13, 4.15, 4.16, 4.17
Dual-porosity formulation	3.3.7	4.7
Double-porosity/double-permeability formulation	3.3.8	4.5
Stress-dependent properties	3.3.9	To be developed
Variable thermal conductivity	3.3.10	To be developed

Table 1. Functional requirements of the FEHM application (continued)

Requirement	Chp. I Section	Tested by (Chp. III section [‡])
Compute solution to transient equations	3.4	4.2, 4.3, 4.4, 4.5, 4.6, 4.7, 4.8, 4.9, 4.10, 4.11, 4.12, 4.13, 4.14, 4.15, 4.16, 4.17
Implement time-step mechanism	3.4.1	
Solve nonlinear equation set at each time step	3.4.2	
Provide input/output data files	3.5	4.2, 4.3, 4.4, 4.5, 4.6, 4.7, 4.8, 4.9, 4.10, 4.11, 4.12, 4.13, 4.14, 4.15, 4.16, 4.17
Inputs	3.4.2	
Outputs	3.4.4	
Provide restart capability	3.6	
Write information needed for restart to output file	3.6.1	4.17
Read information needed for restart from restart file	3.6.2	4.10, 4.17
Resume the calculation	3.6.3	4.10, 4.17
[‡] Chapter III sections (Verification and Validation Plan) 4.1 Testing of Thermodynamic Functions 4.2 Test of Heat Conduction 4.3 Test of Temperature in a Wellbore 4.4 Test of Pressure Transient Analysis 4.5 Test of Infiltration into a One-dimensional, Layered, Unsaturated Medium 4.6 Test of Vapor Extraction from an Unsaturated Reservoir 4.7 Test of Dual Porosity 4.8 Test of Heat and Mass Transfer in Porous Media 4.9 Test of Toronyi Two-phase Problem 4.10 Test of DOE Code Comparison Project, Problem Five, Case A 4.11 Test of Dry-out of a Partially Saturated Medium 4.12 Test of One-dimensional Reactive-Solute Transport 4.13 Test of Henry's Law Species 4.14 Test of Fracture Transport with Matrix Diffusion 4.15 Test of the Movement of a Dissolved Mineral Front 4.16 Test of Multisolute Transport with Chemical Reaction 4.17 Test of Three-dimensional Radionuclide Transport		

Table 2. FEHM macro control statements used by test problems

Control statement	User's Manual [†] section	Used by (Chp. III section) (see footnote in Table I)
adif	6.2.3	Not used
airwater	6.2.4	4.6, 4.13, 4.17
alti	6.2.5	Not used
boun	6.2.6	Not used
bous	6.2.7	Not used
cap	6.2.8	No longer used, see macro rlp
cond	6.2.9	4.2, 4.3, 4.4, 4.6, 4.7, 4.8, 4.9, 4.10, 4.11, 4.12, 4.13, 4.14, 4.15, 4.16, 4.17
cont	6.2.10	4.2, 4.3, 4.4, 4.5, 4.6, 4.8, 4.9, 4.10, 4.11, 4.13, 4.15
coor	6.2.11	4.2, 4.3, 4.4, 4.5, 4.6, 4.7, 4.8, 4.9, 4.10, 4.11, 4.12, 4.13, 4.14, 4.15, 4.16, 4.17
ctrl	6.2.12	4.2, 4.3, 4.4, 4.5, 4.6, 4.7, 4.8, 4.9, 4.10, 4.11, 4.12, 4.13, 4.14, 4.15, 4.16, 4.17
dof	6.2.13	Not implemented
dpdp	6.2.14	4.5
dual	6.2.15	4.7
elem	6.2.16	4.2, 4.3, 4.4, 4.5, 4.6, 4.7, 4.8, 4.9, 4.10, 4.11, 4.12, 4.13, 4.14, 4.15, 4.16, 4.17
eos	6.2.17	Not used
exrl	6.2.18	Not used
finv	6.2.19	4.2
flow	6.2.20	4.2, 4.3, 4.4, 4.5, 4.6, 4.7, 4.8, 4.9, 4.10, 4.11, 4.12, 4.13, 4.14, 4.15, 4.16, 4.17
flo2	6.2.21	Not used
flxo	6.2.22	Not used
head	6.2.23	Not used
hflx	6.2.24	4.11
ice	6.2.25	Not used
init	6.2.26	4.2, 4.3, 4.4, 4.7, 4.8, 4.9, 4.10, 4.12, 4.14, 4.15, 4.16, 4.17
iter	6.2.27	4.5, 4.6, 4.7, 4.11, 4.15, 4.16, 4.17
itup	6.2.28	4.11, 4.17
iupk	6.2.29	Not used
ivfc	6.2.30	Not used
mdnode	6.2.31	Not used

Table 2. FEHM macro control statements used by test problems (continued)

Control statement	User's Manual[†] section	Used by (Chp. III section) (see footnote in Table I)
ngas	6.2.32	4.11
nod2	6.2.33	Not used
node	6.2.34	4.2, 4.3, 4.4, 4.5, 4.6, 4.7, 4.8, 4.9, 4.10, 4.11, 4.12, 4.13, 4.14, 4.15, 4.16, 4.17
perm	6.2.35	4.2, 4.3, 4.4, 4.5, 4.6, 4.7, 4.8, 4.9, 4.10, 4.11, 4.12, 4.13, 4.14, 4.15, 4.16, 4.17
pest	6.2.36	Not used
ppor	6.2.37	Not used
pres	6.2.38	4.5, 4.6, 4.9, 4.11, 4.13, 4.17
ptrk	6.2.39	Not used
renm	6.2.40	Not used
rflx	6.2.41	Not used
rlp	6.2.42	4.5, 4.6, 4.9, 4.10, 4.11, 4.13, 4.17
rock	6.2.43	4.2, 4.3, 4.4, 4.5, 4.6, 4.7, 4.8, 4.9, 4.10, 4.11, 4.12, 4.13, 4.14, 4.15, 4.16, 4.17
rxn	6.2.44	4.13, 4.15, 4.16, 4.17
sol	6.2.45	4.2, 4.3, 4.4, 4.5, 4.6, 4.7, 4.8, 4.9, 4.10, 4.11, 4.12, 4.13, 4.14, 4.15, 4.16, 4.17
solv	6.2.46	Not implemented
stea	6.2.47	Not used
stop	6.2.48	4.2, 4.3, 4.4, 4.5, 4.6, 4.7, 4.8, 4.9, 4.10, 4.11, 4.12, 4.13, 4.14, 4.15, 4.16, 4.17
strs	6.2.49	Not implemented in this version of FEHM
svar	6.2.50	Not used
text	6.2.51	4.5, 4.17
thic	6.2.52	Not used
time	6.2.53	4.2, 4.3, 4.4, 4.5, 4.6, 4.7, 4.8, 4.9, 4.10, 4.11, 4.12, 4.13, 4.14, 4.15, 4.16, 4.17
trac	6.2.54	4.12, 4.13, 4.14, 4.15, 4.16, 4.17
user	6.2.55	Not used
vcon	6.2.56	Not used
velo	6.2.57	Not used

Table 2. FEHM macro control statements used by test problems (continued)

Control statement	User's Manual[‡] section	Used by (Chp. III section) (see footnote in Table I)
wlbr	6.2.58	Not used
zone	6.2.59	4.2, 4.3, 4.5, 4.8, 4.17
#	6.1.1.2	4.5, 4.6, 4.13
file	6.2.2	Not used

[‡]Zyvoloski et al. (1997b)