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MSTS

MULTIPHASE SUBSURFACE TRANSPORT SIMULATOR
USER'S GUIDE AND REFERENCE

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Preface

This User's Guide and Reference is a software document written to provide instructions and a detailed reference necessary to use the Multiphase Subsurface Transport Simulator (MSTS) and a closely associated utility, the MSTS Graphical Input. The design architecture and specific computational algorithms that compose MSTS are delineated in a companion document, the MSTS Theory Manual.

It is assumed in writing this User's Guide and Reference that the user of this code has received advanced training in hydrogeology, heat transfer, and thermodynamics. It is also assumed that users are familiar with the computing environment in which they will compile and use the MSTS code.

Machine requirements for the MSTS code are dependent on the nature of the problem to be solved. The MSTS code is not machine-dependent, and with essentially minor changes (detailed in this User's Guide and Reference), the MSTS code may be compiled and run on many different computer environments using a FORTRAN 77 compiler. Naturally, the speed with which problems are solved depends on the capacity and speed of the computing platform and the size of the problem. Small one-dimensional problems may be solved quickly on a desktop computer, but large, complex two- or three-dimensional multiphase problems may be practically tackled only using a workstation or mainframe. The MSTS Graphical Input may be used only with a Macintosh computer.

Summary

This User's Guide and Reference provides information and instructions on the use of the Multiphase Subsurface Transport Simulator (MSTS) code and the associated MSTS Graphical Input. The MSTS code is used to simulate water flow, air flow, heat transfer, and dilute species mass transport in variably saturated geologic media for one, two, or three dimensions using an integrated finite-difference numerical scheme. Any or all of these processes may be simulated in a fully coupled manner. MSTS is a two-phase, two-component code with secondary processes that include binary diffusion and vapor pressure lowering. The geologic media may be homogeneous or heterogeneous, isotropic or anisotropic, and unfractured or highly fractured. A problem geometry may be described by either Cartesian or cylindrical coordinates. MSTS is written in FORTRAN 77, following the American National Standards Institute (ANSI) standards, and is machine-independent with the exception of some time and date calls required for quality control (provisions are made in the code for relatively easy adaption to a number of machines for these calls).

KEYWORDS: multiphase, ground-water flow, multiple phase, variably saturated, unsaturated, finite difference, numerical modeling, Newton-Raphson iteration, equivalent-continuum model.

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Glossary of Symbols

Roman Symbols

Symbol	Description	Dimensions	SI[a] Units
A, A_ℓ, A_g	function curve-fitting parameters	-	-
B, B_ℓ, B_g	function curve-fitting parameters	-	-
c_s	specific heat capacity of solid phase	$L^2\ t^{-2}\ T^{-1}$	J/kg K
C, C_ℓ, C_g	species concentration (per total volume, per aqueous volume, per gas volume)	mol L^{-3}	mol/m^3
Cr	Courant Number	-	-
D	diffusion conductance	mol $L^{-2}\ t^{-1}$	mol/m^2 s
D_g^{aw}	air water-vapor binary diffusivity	$L^2\ t^{-1}$	m^2/s
$\tilde{D}_{h_\ell}$	species hydraulic-dispersion coefficient (aqueous)	$L^2\ t^{-1}$	m^2/s
D_{d_ℓ}, D_{d_g}	species diffusion coefficient (aqueous, gas)	$L^2\ t^{-1}$	m^2/s
g	acceleration of gravity	$L\ t^{-2}$	m/s^2
h_ℓ, h_g	enthalpy (aqueous, gas)	$L^2\ t^{-2}$	J/kg
h^w, h^a	enthalpy (water, air)	$L^2\ t^{-2}$	J/kg
H_T, H_E, H_p	hydraulic head (total, elevational, pressure)	L	m
$\tilde{k}$	intrinsic permeability tensor	L^2	m^2
$k_{r\ell}, k_{rg}$	relative permeability (aqueous, gas)	-	-
$k_{r\ell_b}, k_{r\ell_f}, k_{r\ell_m}$	aqueous relative permeability (bulk, fracture, matrix)	-	-

(a) Système International

Roman Symbols (Contd)

Symbol	Description	Dimensions	SI Units
$\tilde{k}_e$	effective thermal conductivity tensor	M L t^{-2} T^{-1}	W/m K
K_d	partition coefficient (solid-aqueous systems)	-	-
$K_{\ell g}$	partition coefficient (aqueous-gas systems)	-	-
m	moisture-retention curve-fitting parameter	-	-
m_f, m_m	moisture-retention curve-fitting parameter (fracture, matrix)	-	-
m_ℓ^w, m_g^w	water mass (aqueous, gas phases)	M	kg
$\dot{m}^w$, $\dot{m}^a$	mass source rate per volume (water, air)	M L^{-3} t^{-1}	kg/m^3 s
$\dot{m}_\ell$, $\dot{m}_g$	mass source rate (aqueous, gas)	M t^{-1}	kg/s
n	moisture-retention curve-fitting parameter	-	-
n_f, n_m	moisture-retention curve-fitting parameter (fracture, matrix)	-	-
n_D, n_E, n_T	porosity (diffusive, effective, total)	-	-
n_{D_f}, n_{E_f}, n_{T_f}	fracture porosity (diffusive, effective, total)	-	-
n_{D_m}, n_{E_m}, n_{T_m}	matrix porosity (diffusive, effective, total)	-	-
P_ℓ, P_g	pressure (liquid, gas)	M L^{-1} t^{-2}	Pa
P_{cap}	capillary pressure	M L^{-1} t^{-2}	Pa
Pe	Peclet Number	-	-
q	thermal energy	M L^2 t^{-2}	J

Roman Symbols (Contd)

Symbol	Description	Dimensions	SI Units
$\dot{q}$	thermal energy source power density	$M\ L^2\ t^{-3}$	W/m^3
$\dot{Q}_e$	thermal energy flux rate	$M\ t^{-3}$	W/m^2
$\dot{Q}_c$	species flux rate	$mol\ L^{-2}\ t^{-1}$	$mol/m^2\ s$
$\dot{Q}_\ell, \dot{Q}_g$	mass flux rate (aqueous, gas phases)	$M\ L^{-2}\ t^{-1}$	$kg/m^2\ s$
r	radial coordinate (cylindrical coordinate systems)	radians	radians
r_0	inner radius of model domain (cylindrical coordinate systems)	radians	radians
R^w, R^a	ideal gas constant (water, air)	$L^2\ t^{-2}\ T^{-1}$	J/kg K
$\dot{R}_c$	species decay rate	t^{-1}	1/s
$\dot{s}_c$	species source (mass basis)	$mol\ L^{-3}\ t^{-1}$	mol/ s
$\dot{s}_{c,v}$	species source (concentration basis)	$mol\ L^{-3}\ t^{-1}$	$mol/m^3\ s$
s_ℓ, s_g	saturation (aqueous, gas)	-	-
$s_{\ell_b}, s_{\ell_f}, s_{\ell_m}$	aqueous saturation (bulk, fracture, matrix)	-	-
s_ℓ^*	effective aqueous saturation	-	-
$s_{\ell r}$	residual aqueous saturation	-	-
$s_{\ell r_f}, s_{\ell r_m}$	residual aqueous saturation (fracture, matrix)	-	-
s_{sr}	entrapped air saturation	-	-
S_s	coefficient of specific storage	L^{-1}	1/m
t	time	t	s
T	temperature	T	°C or K

Roman Symbols (Contd)

Symbol	Description	Dimensions	SI Units
u_s	solid-phase internal energy	$L^2\ t^{-2}$	J/kg
u_g^w, u_g^a	gas-phase internal energy (water, air)	$L^2\ t^{-2}$	J/kg
u_ℓ^w, u_ℓ^a	aqueous-phase internal energy (water, air)	$L^2\ t^{-2}$	J/kg
u	east-west Darcy velocity	$L\ t^{-1}$	m
V	volume	L^3	m^3
$\mathbf{V}_\ell, \mathbf{V}_g$	phase velocity (aqueous, gas)	$L\ t^{-1}$	m/s
v	south-north Darcy velocity	$L\ t^{-1}$	m/s
w	bottom-top Darcy velocity	$L\ t^{-1}$	m/s
x	west-east coordinate (Cartesian coordinate systems)	L	m
x_g^w, x_g^a	gas-phase mass fraction (water, air)	-	-
x_ℓ^w, x_ℓ^a	aqueous-phase mass fraction (water, air)	-	-
y	south-north coordinate (Cartesian coordinate systems)	L	m
z	bottom-top coordinate (Cartesian and cylindrical coordinate systems)	L	m
$\hat{z}$	elevational gradient	$L\ L^{-1}$	m/m
z^*	datum elevation	L	m

Greek Symbols

Symbol	Description	Dimensions	SI Units
α	moisture-retention curve-fitting parameter	L^{-1}	1/m
α_f, α_m	moisture-retention curve-fitting parameter (fracture, matrix)	L^{-1}	1/m
β	moisture-retention curve-fitting parameter	-	-
η_D	total water content	$L^3\ L^{-3}$	m^3/m^3
θ	volumetric moisture content	$L^3\ L^{-3}$	m^3/m^3
θ_r	residual moisture content	$L^3\ L^{-3}$	m^3/m^3
θ_s	saturated moisture content	$L^3\ L^{-3}$	m^3/m^3
θ	angular coordinate (cylindrical coordinate systems)	radians	radians
μ_g^w, μ_g^a	gas-phase component viscosity (water, air)	$M\ L^{-1}\ t^{-2}$	Pa s
μ_ℓ, μ_g	viscosity (aqueous, gas)	$M\ L^{-1}\ t^{-2}$	Pa s
ρ_ℓ, ρ_g, ρ_s	mass density (aqueous, gas, solid)	$M\ L^{-3}$	kg/m^3
σ^{aw}	air-water surface tension	$M\ t^{-2}$	N/m
τ_ℓ, τ_g	tortuosity (aqueous, gas)	-	-
χ_ℓ^a, χ_g^a	mole fraction of air (aqueous, gas)	-	-
ψ	tension head (negative pressure head)	L	m
ψ^*	minimum drainage capillary pressure head	L	m

Subscripts

Symbol	Description
cap	capillary
D	diffusive
e	equivalent
E	effective
f	fracture
g	gas phase
ℓ	aqueous phase
r	residual
s	solid phase; saturation state
T	total

Superscripts, Overscripts

Symbol	Description
~	tensor
*	reference value; effective

Mathematical Symbols

Symbol	Description
∇	divergence operator
∂	partial differential operator
( )	function operator
| |	absolute value operator
ln(x)	natural logarithm of variable x

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1.0 Introduction

The Multiphase Subsurface Transport Simulator (MSTS) is a numerical model and computer code capable of solving fully coupled equations for conservation of water and air mass, conservation of energy, and conservation of dilute species mass in variably saturated geologic media. MSTS employs an integrated finite-difference numerical scheme in conjunction with a Newton-Raphson iteration scheme to solve the coupled equations for water conservation, air conservation, and energy conservation. The species solute mass conservation equation is solved sequentially to the coupled governing equations with a direct integrated finite-difference scheme. One-, two-, or three-dimensional domains may be simulated in a time-transient fashion.

The MSTS Graphical Input is an extremely useful pre-processor for preparing the input files that direct MSTS simulations. The interface uses a "point-and-click" approach to speed entry of geometry specification, numerical solution control, boundary and initial conditions, output directions, and geologic property values. The MSTS Graphical Input also provides elementary error checking and determines the minimum size of MSTS FORTRAN parameters required for an MSTS input file. A distinct advantage of using the MSTS Graphical Input is that this pre-processor observes all of the input file format requirements, removing the burden from the code user of learning the input file structure and constantly adhering to it.

MSTS and the MSTS Graphical Input were developed by Pacific Northwest Laboratory[a] at the request of the Yucca Mountain Project Office of the U.S. Department of Energy to produce numerical predictions of subsurface flow and transport phenomena at the potential high-level nuclear waste repository site at Yucca Mountain, Nevada.

This document is designed to introduce the user to the MSTS code, demonstrate its use, and provide a comprehensive reference of input commands used to build an MSTS input file. New users can follow the "Quick Tour" (Section 5.0) to see, step by step, how to build an input file and run a small, one-dimensional simulation. Finally, input files and results are provided for a variety of example problems to demonstrate the range of MSTS applications. Several of these example problems double as test problems, with the results compared either to analytic solutions or to other computer models. The design architecture and specific computational algorithms that compose MSTS are delineated in a companion document, the MSTS Theory Manual (White and Nichols 1992).

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2.0 MSTS Capabilities Overview

The Multiphase Subsurface Transport Simulator can solve a wide variety of single- or multiple-phase problems for unsaturated or saturated geologic media. The four basic governing equations it solves are conservation of water mass, conservation of air mass, conservation of thermal energy, and conservation of a dilute species mass. In this overview, the main features of the MSTS code are introduced and the fundamental governing equations are presented. Additional details on the mathematical basis and theory of the MSTS code are available in the MSTS Theory Manual (White and Nichols 1992).

2.1 Main Features of MSTS

By the appropriate use of the features of the MSTS computer code, a wide range of porous media problems can be solved. This section provides a brief overview of the major features of MSTS. More detailed information on the use of these features is discussed in subsequent sections of this document.

2.1.1 Spatial Dimensionality and Coordinate Systems

MSTS is designed to solve one-, two-, or three-dimensional problems. A problem can be defined and solved using either Cartesian or cylindrical coordinates. In a Cartesian coordinate problem, the horizontal plane is represented by x-y coordinates, but for cylindrical problems the horizontal plane is represented by r-θ coordinates. The vertical coordinate, coincident with the gravity vector, is represented by z in both coordinate systems.

2.1.2 Time and Space Dependence

All MSTS solutions are time-dependent (transient); steady-state solutions are obtained with MSTS either directly or with false transients. The values of certain parameters (e.g., sources of fluid or gas mass, thermal energy, or species mass) can be varied in time. Time-varying inputs are specified in tabular format. Time variance in parameters such as boundary conditions that are constant in time can be accommodated through use of the restart feature in MSTS.

All physical properties of a porous medium can be spatially varied by rock or soil type to model heterogeneity. There are no limits, within computer memory constraints, to the number of rock or soil types that can be defined. Certain physical properties, such as thermal or hydraulic conductivity, can be anisotropic.

2.1.3 Equation Coupling

Three of the four governing equations solved by MSTS–water conservation, gas conservation, and thermal energy conservation–are solved in a fully coupled manner. The fourth equation, dilute species mass conservation, is solved sequentially to the other governing equations. Depending on the nature of the problem, any or all of the four governing equations may be activated for a particular simulation. Hence, problems that are concerned only with isothermal fluid flow would require activating only the water conservation equation. Problems involving contaminant transport in an isothermal, fully saturated environment would require solution of only the water mass conservation and species mass conservation equations.

2.1.4 Boundary Conditions

Boundary conditions that can be specified using MSTS include Dirichlet, Neumann, saturated, and unit-gradient conditions as applicable to each physical process. Boundaries can be defined over an entire surface, over some smaller portion of a surface, or at the interface between computational nodes and internal "inactive" (noncomputational) nodes. Boundaries are separately defined for aqueous-phase mass, gas-phase mass, vapor mass, thermal energy, and species mass.

2.1.5 Solution Methods for Governing Equations

Governing equations are solved by discretizing the governing equations over the spatial grid for a discrete time step and solving the resulting system of nonlinear algebraic equations. Nonlinearities in the discretized governing equations are resolved with Newton-Raphson iteration. Either a banded matrix or conjugate gradient solution scheme may be used. Where iteration is required to obtain a solution, the Newton-Raphson technique is employed.

2.1.6 Operational Control

Operational control is exercised by means of commands included in the input file that specify the length of simulation, time-step control, solution techniques, which of the governing equations to solve, convergence criteria for each governing equation, wallclock and CPU time limits for the simulation execution, and other aspects of simulation control. A restart capability is incorporated into MSTS to add additional flexibility.

2.1.7 Output Control

Output is controlled through use of commands included in the input file that permit a user to specify which field variables are recorded at which simulation steps and for which grid nodes. Output is separately controlled for the general output file, the plot file (which may be used with a

variety of third-party graphical post-processors), and reference node output that is produced during simulation execution.

2.1.8 Variable Saturation

The numerical solution scheme employed in MSTS allows the solution of fluid flow in both the vadose (unsaturated) zone and the fully saturated domain. In the vadose zone, solution of the water conservation equation alone assumes that liquid water and gas (air) exist, but only liquid-phase movement is modeled. If both the water and gas conservation equations are activated, then both water and gas motion is modeled.

2.1.9 Porosity

The MSTS code is based on a three-porosity conceptual model of porous media. These porosities are termed effective, total, and diffusive. Effective, or kinematic, porosity (n_E) is the ratio of the volume of void space in a representative elementary volume (REV) through which water effectively advects to the total volume of the REV. Total porosity (n_T) is the ratio of the volume of void space of a REV to the total volume of the REV. Diffusive porosity (n_D) is the ratio of the volume of connected pore space to the total volume of the REV. Effective, diffusive, and total porosity are always subject to the physical constraint, $n_E \leq n_D \leq n_T$.

2.1.10 Sources and Sinks

Sources and sinks of thermal energy, water mass, gas mass, and dilute species mass may be included in an MSTS simulation. The strength of a source or sink either may be constant over prescribed time periods or may vary in time following a tabular specification. A source or sink is defined in relation to a node or range of nodes, giving spatial variability as required.

2.1.11 Graphical Input

A closely knit application that enhances the use of MSTS is the MSTS Graphical Input, a graphical user interface that makes preparation and modification of consistent, format-error-free input files radically easier than for previous hydrogeologic codes. The Graphical Input application was available for the Macintosh at the time this document was written, but versions for other computing environments may be available; check the "read.me" file on any distribution diskettes for more recent information.

2.1.12 Units

MSTS performs all internal calculations using Système International (SI) units; all data and parameters are handled strictly in SI units. However, to allow for easy data entry, MSTS will read a wide variety of units from input files, including SI-derived units and English Engineering units. It accomplishes this by converting all input to SI units as it is imported. Hence, most information can be entered in the units in which it was originally recorded, while the advantages of working with SI units are retained.

2.2 Application Scope

The four fundamental equations for conservation of component mass, energy, and species mass that compose MSTS essentially define the simulator's application scope. A fundamental restriction with respect to MSTS's application scope is that all applications are strictly limited to subsurface porous media environments. This restriction holds because of the application of Darcy's law to compute phase volumetric fluxes. Furthermore, driving forces for fluid flow are limited to pressure gradients and gravitational body forces. MSTS is classified as a two-component, two-phase simulator. This classification indicates that the simulator is capable of computing flow and transport processes for subsurface systems that contain no more than two components and two phases. Moreover, components are confined to water and air, and phases are confined to aqueous and gas. Subsurface systems contaminated with significant concentrations of an organic compound fall outside of MSTS's application scope. Low solubilities are assumed in expressing the quantity of air dissolved in the aqueous phase. Within the gas phase, component mass fractions are completely variable. Liquid saturations and relative permeabilities are computed neglecting hysteretic and air entrapment effects. The flow model for highly fractured systems assumes that the porous medium and the fractures are continuously in thermal and hydraulic equilibrium. Although discrete fractures can be modeled with MSTS, the simulator is inappropriate for modeling transient fracture-matrix interactions with the dual-porosity model.

The energy conservation equation expands the application scope by allowing thermal gradients to influence the flow fields. The energy equation formulation allows for both sensible and latent heat transfer. Sensible heat transfer occurs by thermal diffusion through the solid and aqueous phases and by advection through the aqueous phase. Diffusive heat transfer through the gas phase is neglected. Latent heat transfer by evaporation and condensation processes is considered for the water component. Because interphase mass transfer computations depend on the assumption of thermodynamic equilibrium, MSTS is not applicable for systems requiring disequilibrium or kinetic

modeling of the thermodynamic processes. Sensible and latent heat transfer associated with diffusing or dispersing components is neglected. Therefore, enhanced heat transfer by vapor migration under thermal gradient conditions must be included empirically into the effective thermal conductivity coefficient.

Species transport processes are solved by assuming loose coupling between multiphase fluid flow and species transport processes. Because of the strong dependence of phase pressures and temperature on the secondary variables that compose the fundamental equations for mass and energy conservation, these fluid flow and heat transport fundamental equations are solved simultaneously (coupled). The principal assumption associated with the species transport processes is that the species are numerically considered passive scalars. Physically, this assumption implies that the secondary variables of the mass and energy conservation equations are independent of species concentrations. A passive scalar species limits the applicability of the engineering simulator to dilute species concentrations. Species concentrations may be considered dilute whenever the physical, thermal, or transport properties of the transport fluid remain unaltered. The dilute concentration assumption and decoupled solution approach also allow consideration of multiple species and transport modeling of radioactive decay products. No accounting is made of chemical reaction and/or radioactive decay products.

2.3 Governing Equations

MSTS employs four partial differential equations as the governing equations to mathematically describe the transport of water, air, thermal energy, and a dilute species in the subsurface environment. Each partial differential equation represents an expression of conservation for either component mass, thermal energy, or the species mass. The conservation equations balance the time rate of change in the conserved quantity within a control volume against the surface fluxes of the conserved quantity entering or leaving the control volume. The conserved quantities are water mass, air mass, thermal energy, and species mass. Transport of the four conserved quantities through a porous medium is modeled within two distinct phases: aqueous and gas. The aqueous phase is composed primarily of water, with relatively small amounts of dissolved air, whereas the gas phase is composed of various compositions of air and water vapor.

2.3.1 Water Mass Conservation Equation

The conservation equation for water mass, expressed in partial differential equation form, is shown in Equation (2.1). The term on the left-hand side of Equation (2.1) represents the time rate of change of water mass within the control volume. Water occurs within the soil pores as liquid in

the aqueous phase and as vapor in the gas phase. Unconnected pore spaces are considered to be filled with liquid water but isolated from the continuous pore spaces, and therefore do not contribute to the water mass accumulation term. Interphase mass transfer of water between the aqueous and gas phases is computed by assuming thermodynamic equilibrium conditions. This equilibrium assumption implies that time scales for thermodynamic processes are significantly shorter than for those associated with transport. The two gradient terms on the right-hand side of Equation (2.1) represent the net mass flux of water mass into the control volume through the aqueous and gas phases, respectively. Water mass flux occurs by advection in both phases and by diffusion through the gas phase. Advective transport is governed by Darcy's law for flow through porous media, where phase pressure gradients and gravitational forces drive the flow fields. For unsaturated porous media, advective transport depends on saturation-dependent relative permeabilities for each phase. Component diffusion rates through the aqueous phase are neglected as a transport mechanism. Diffusion through the gas phase is governed by the classical mass diffusion equation, modified by the porous media tortuosity. The driving forces behind diffusive transport are component concentration or mass fraction gradients in the gas phase. The last term on the right-hand side of Equation (2.1) represents the water mass source rate within the control volume.

$$\frac{\partial}{\partial t}\left[n_D x_\ell^w \rho_\ell s_\ell + n_D x_g^w \rho_g s_g\right] = \nabla\left[\frac{x_\ell^w \tilde{k} k_{r\ell} \rho_\ell}{\mu_\ell}\left(\nabla P_\ell + \rho_\ell g \hat{z}\right)\right] + \nabla\left[\frac{x_g^w \tilde{k} k_{rg} \rho_g}{\mu_g}\left(\nabla P_g + \rho_g g \hat{z}\right) + \tau_g n_D \rho_g s_g D_g^{aw} \nabla x_g^w\right] + \dot{m}^w \tag{2.1}$$

2.3.2 Air Mass Conservation Equation

The conservation equation for air mass, expressed in partial differential equation form, is shown in Equation (2.2). The term on the left-hand side of Equation (2.2) represents the time rate of change of air mass in the control volume. Air occurs within the soil pores as dissolved air in the aqueous phase and as gaseous air the gas phase. Occluded air within the aqueous phase is neglected, by assuming that air entrapped by imbibing water would eventually dissolve into the aqueous phase. Unconnected pore spaces are considered to be filled with liquid water, but isolated

from the continuous pore spaces, and therefore do not contribute to the air mass accumulation term. Interphase mass transfer of air between the aqueous and gas phases is computed by assuming thermodynamic equilibrium conditions. This equilibrium assumption implies that time scales for thermodynamic processes are significantly shorter than for those associated with transport. The two gradient terms on the right-hand side of Equation (2.2) represent the mass flux of air mass into the control volume through the aqueous and gas phases, respectively. Air mass flux occurs by advection in both phases and by diffusion through the gas phase. Advective transport is governed by Darcy's law for flow through porous media, where phase pressure gradients and gravitational forces drive the flow fields. For unsaturated porous media, advective transport depends on saturation-dependent relative permeabilities for each phase. Component diffusion rates through the aqueous phase are neglected as a transport mechanism. Diffusion through the gas phase is governed by the classical mass diffusion equation, modified by the porous media tortuosity. The driving forces behind diffusive transport are component concentration or mass fraction gradients in the gas phase. The last term on the right-hand side of Equation (2.2) represents the air mass source rate within the control volume.

$$\frac{\partial}{\partial t}\left[n_D x_\ell^a \rho_\ell s_\ell + n_D x_g^a \rho_g s_g \right] = \nabla\left[\frac{x_\ell^a \tilde{k} k_{r\ell} \rho_\ell}{\mu_\ell}\left(\nabla P_\ell + \rho_\ell g \hat{z}\right)\right] + \nabla\left[\frac{x_g^a \tilde{k} k_{rg} \rho_g}{\mu_g}\left(\nabla P_g + \rho_g g \hat{z}\right) - \tau_g n_D \rho_g s_g D_g^{aw} \nabla x_g^w \right] + \dot{m}^a \tag{2.2}$$

2.3.3 Thermal Energy Conservation Equation

The conservation equation for thermal energy, expressed in partial differential form, is shown in Equation (2.3), where phase velocities are defined by Equations (2.4) and (2.5) for the aqueous and gas phases, respectively. The term on the left-hand side of Equation (2.3) represents the time rate of change of heat content in the control volume. The total heat contained in the control volume depends directly on temperature, liquid saturations, phase compositions, and soil physical properties. For the thermal energy conservation equation, a modified aqueous-phase saturation applies that accounts for the thermal capacitance of unconnected pore spaces, which are assumed to

be filled with liquid water. Internal energies and densities of the aqueous phase are those for pure liquid water. This assumption follows directly from the principal assumption of relatively low solubilities of air in the aqueous phase. Disparately, the internal energy of the gas phase is strongly dependent on phase composition. The first term on the right-hand side of Equation (2.3) represents heat transfer into the control volume by advection. Analogous to the evaluation of internal energies, the enthalpy of the aqueous phase is that for pure liquid water, whereas the gas-phase enthalpy is strongly dependent on phase composition. The second term on the right-hand side of Equation (2.3) represents heat transfer by conduction and mechanical dispersion. The equivalent conductivity tensor represents the combination of solid- and liquid-phase conductivities along with the mechanical dispersion coefficient. Typically, the mechanical dispersion tensor is neglected by assigning zero to the longitudinal and transverse dispersivities. Thermal conductivity through the gas phase is neglected. The last three terms on the right-hand side of Equation (2.3) represent internal heat generation quantities from thermal energy sources and sinks within the control volume, and the change in internal energy associated with water and air mass sources and sinks within the control volume, respectively. The internal heat generation from mass sources represent the enthalpy associated with a mass source.

$$\frac{\partial}{\partial t}\left[\left(1-n_T\right)\rho_s u_s+\eta_D\,\rho_\ell u_\ell+n_D\,s_g\,\rho_g\,u_g\right]= \tag{2.3}$$

$$-\nabla\left[\rho_\ell h_\ell \mathbf{V}_\ell+\rho_g h_g \mathbf{V}_g\right]+\nabla\left[\tilde{k}_e \nabla T\right]+\dot{q}+h^w \dot{m}^w+h^a \dot{m}^a$$

where

$$\mathbf{V}_\ell = A\,\frac{\tilde{k}\,k_{r\ell}}{\mu_\ell}\left(\nabla P_\ell+\rho_\ell g\,\hat{z}\right) \tag{2.4}$$

$$\mathbf{V}_g = A\,\frac{\tilde{k}\,k_{rg}}{\mu_g}\left(\nabla P_g+\rho_g g\,\hat{z}\right) \tag{2.5}$$

2.3.4 Species Mass Conservation Equation

The conservation equation for species mass, expressed in partial differential equation form, is shown in Equation (2.6). The term on the left-hand side of Equation (2.6) represents the time rate of change of total species mass within a control volume. Interphase species mass transfer between solid and fluid phases is computed by assuming that thermodynamic and geochemical equilibrium conditions apply. This assumption of equilibrium conditions requires that time scales for thermodynamic and geochemical phenomena be small when compared with those for transport phenomena. For transport through geologic media, these assumptions are generally appropriate. The first term on the right-hand side of Equation (2.6) represents the migration of species mass into the control volume by advection through the aqueous and gas phases. Advective transport is dependent on the species concentration and Darcy velocity within each phase. The second term on the right-hand side of Equation (2.6) represents the hydrodynamic dispersion of species in the aqueous phase. The third term on the right-hand side of Equation (2.6) represents the diffusion of species mass into the control volume in the aqueous and gas phases. Typically, diffusion coefficients for the gas phase will be several orders of magnitude greater than those for the aqueous phase. Species diffusion fluxes are phase specific and depend on the gradients in species phase concentrations, phase pore areas, and phase tortuosities. The fourth term on the right-hand side of Equation (2.6) represents the generation of species within the control volume. The last term on the right-hand side of Equation (2.6) represents the radioactive decay or consumption rate of species mass.

$$\frac{\partial C}{\partial t} = -\nabla\left[C_\ell \mathbf{V}_\ell + C_g \mathbf{V}_g \right] + \nabla\left[s_\ell n_D \tilde{D}_{h_\ell} \nabla C_\ell \right] + \nabla\left[\tau_\ell s_\ell n_D D_{d_\ell} \nabla C_\ell + \tau_g s_g n_D D_{d_g} \nabla C_g \right] + \dot{s}_c - \dot{R}_c C \tag{2.6}$$

2.4 Solution Options

One of the design goals for MSTS was to create an efficient numerical simulator for predicting flow and transport phenomena in the subsurface environment. Because of the diversity of subsurface flow problems, a single-solution option would result in a numerical simulator that was computationally inefficient for a majority of problems. For example, if the simulation problem involved generating predictions of radionuclide transport by ground water under isothermal

conditions, then it would be superfluous to include gas-phase transport and heat transfer in the solution scheme. The preferred solution scheme in terms of computational efficiency would be to sequentially solve the water mass conservation and species mass conservation equations. However, if the simulation problem involves nonisothermal aspects and if species transport through the gas phase is significant, then the solution scheme would require the coupled solution of both component mass conservation equations and the energy equation, along with the sequential solution of the species transport equation. To avoid simulating the negligible aspects of a particular subsurface flow and transport problem, several solution options are available with MSTS. This approach yields a simulator that depends on the problem characteristics.

Solution modes or options are characterized by the specific solved conservation equations. The conservation equations are divided into coupled and auxiliary conservation equations according to their interdependencies. The governing conservation equations for water mass, air mass, and energy are considered coupled equations because they are solved simultaneously. The species mass conservation equation is considered an auxiliary equation because it is solved sequentially to the coupled conservation equations. The lowest-order solution modes are those that involve the solution of a single coupled conservation equation (e.g., water mass conservation, air mass conservation, or energy conservation). These lower-order solution modes generally require more assumptions about the subsurface system to be applicable. The next-higher-order solution modes are those that involve the coupled solution of a pair of conservation equations. These solution modes typically eliminate one of the primary assumptions associated with a single-equation solution mode. The highest-order solution mode requires the coupled solution of both component mass conservation equations and the energy conservation equation. The computational effort increases roughly with the square of the coupled equations solved (i.e., three coupled equations require eight times the computational effort required for a single equation). All solution modes can include the solution of the auxiliary species conservation equation.

Solution modes are chosen by the user according to the coupled conservation equations selected for solution. Considerable computational savings may be achieved through the proper choice of a solution mode for a particular application. Choosing lower-order solution modes (i.e., those with fewer equations) generally requires that some assumptions be made about the problem. Some assumptions are obvious (e.g., eliminating the air mass conservation equation for isothermal ground-water flow problems, or eliminating the energy conservation equation for isothermal problems). Other assumptions require previous modeling experience, experimental evidence, or field observations to support the elimination of a specific equation. For example, what thermal gradients constitute the inclusion of vapor transport through the gas phase to accurately predict heat

transfer rates? Answering this type of question requires specific property information about the porous media and anticipated thermal gradients.

The following sections (2.4.1 through 2.4.7) describe the seven solution modes available in MSTS. Each section is labeled with a solution mode title, followed by brief general description of the solution mode and the type of problems to which it applies. Each section also contains primary, secondary, and velocity variable lists. Primary variables refer to the principal unknowns for the solution mode. The number of primary variables and the number of solved equations always coincide. Fixed primary variables refer to primary variables that must be specified according to the problem assumptions. Fixed primary variables are specified, not computed. For example, the gas-phase pressure for a ground-water flow problem solved in the Water mode might be fixed to atmospheric conditions, or 101,325.0 Pa. Secondary variables are physical properties, transport properties, and saturations that are computed from the unknown and fixed primary variables. Fixed secondary variables are physical properties, transport properties, and saturations, required for the solved equations, that are independent of the unknown primary variables. For example, liquid viscosities generally are considered independent of liquid pressures. Velocities refer to flow velocities or diffusion mass fluxes computed by the engineering simulator from the solution of the unknown pressure field. Fixed velocities are those velocities or diffusion mass fluxes computed for inactive phases from fixed pressure fields, soil characteristics, and transport properties.

2.4.1 Water

Description: The Water mode solves saturated and unsaturated ground-water flow problems without a participating gas phase. Soil characteristics are computed for a two-phase air-water system using nonhysteretic relations. Physical properties may be specified invariant or dependent on aqueous pressure. Species transport in the aqueous phase may be modeled by additionally solving the species mass conservation equation.

Application: Appropriate applications for the Water mode include saturated and unsaturated ground-water flow problems with negligible thermal and gas pressure gradients.

Specification: Solution Schemes card

- Governing Equations
  - Thermal Energy Conservation Equation: off
  - Water Conservation Equation: on
  - Air Conservation Equation: off
  - Species Conservation Equation: off / on
- Options
  - Binary Diffusion: off
  - Fixed Properties: off / on
  - Liquid Phase: on
  - Gas Phase: off
  - Vapor Pressure Lowering: off

Primary Variables: aqueous pressure

Fixed Primary Variables: gas pressure, temperature

Secondary Variables: aqueous-phase density, aqueous-phase saturation, aqueous-phase relative permeability, porosity, aqueous-phase tortuosity

Fixed Secondary Variables: aqueous-phase viscosity

Fluxes: aqueous-phase velocity

2.4.2 Air

Description: The Air mode solves unsaturated subsurface gas flow problems with static saturation fields. Liquid saturations are temporally invariant, and are either specified or computed from initial fields of aqueous pressure and gas pressure. Fixed physical properties are temporally invariant, computed from the initial fields of aqueous pressure, gas pressure, and temperature. Vapor diffusive transport and convective mass transport may be computed through the gas phase for spatially variant temperature fields. Conservation of water mass and energy is not ensured for vapor transport problems. Gas-phase density, gas-phase mass fractions, and vapor diffusivities may be specified invariant or dependent on gas pressure. Species transport in the gas phase can be modeled by additionally solving the species mass conservation equation.

Application: Appropriate applications for the Air mode include unsaturated subsurface gas flow problems with invariant liquid saturation and temperature fields. Density-driven gas flows resulting from steady thermal gradients would be an appropriate problem for this mode. For these types of applications, the influence of both temperature and vapor mass fractions on gas-phase properties could be investigated. An inappropriate application, however, would result if either the liquid saturation or the thermal fields were significantly altered by the transport of vapor or heat through the gas phase.

Specification: Solution Schemes card

- Governing Equations
  - Thermal Energy Conservation Equation: off
  - Water Conservation Equation: off
  - Air Conservation Equation: on
  - Species Conservation Equation: off / on
- Options
  - Binary Diffusion: off / on
  - Fixed Properties: off / on
  - Liquid Phase: off
  - Gas Phase: on
  - Vapor Pressure Lowering: off / on

Primary Variables: gas pressure

Fixed Primary Variables: aqueous pressure, temperature

Secondary Variables: water-vapor partial pressure, air partial pressure, water-vapor density, air density, gas-phase density, water-vapor mass/mole fraction, air mass/mole fraction, gas-phase viscosity, water-vapor diffusivity

Fixed Secondary Variables: aqueous-phase saturation

Fluxes: gas-phase velocity, water-vapor diffusion mass flux

2.4.3 Water-Air

Description: The Water-Air mode solves saturated and unsaturated ground-water flow problems with a participating gas phase. Soil characteristics are computed for a two-phase air-water system using nonhysteretic relations. Physical properties are temporally invariant, computed from the initial fields of aqueous pressure, gas pressure, and temperature. Water-vapor transport through the gas phase is computed for spatially variant temperature fields. Phase densities, mass fractions, and vapor diffusivities may be specified invariant or dependent on pressure. Species transport in the aqueous and gas phases can be modeled by additionally solving the species mass conservation equation.

Application: Appropriate applications for the Water-Air mode include saturated and unsaturated ground-water flow problems with steady or negligible thermal gradients. This mode differs from the Water mode because it is applicable to problems involving gas pressure gradients. For steady thermal conditions, this mode is appropriate for predicting the transport of water vapor by diffusion and advection through the gas phase. The mode becomes inappropriate when the liquid and mass transport influences the thermal field. Because heat transfer associated with vaporization and condensation may be significant, thermal effects should be considered carefully before applying this mode to a simulation problem.

Specification: Solution Schemes card

- Governing Equations
  - Thermal Energy Conservation Equation: off
  - Water Conservation Equation: on
  - Air Conservation Equation: on
  - Species Conservation Equation: off / on
- Options
  - Binary Diffusion: off / on
  - Fixed Properties: off / on
  - Liquid Phase: on
  - Gas Phase: on
  - Vapor Pressure Lowering: off / on

Primary Variables: aqueous pressure, gas pressure

Fixed Primary Variables: temperature

Secondary Variables: water-vapor partial pressure, air partial pressure, water-vapor density, air density, gas-phase density, aqueous-phase density, air mass/mole fraction, water-vapor mass/mole fraction, aqueous-phase air mass/mole fraction, gas-phase viscosity, aqueous-phase saturation, gas-phase saturation, aqueous-phase relative permeability, gas-phase relative permeability, porosity, aqueous-phase tortuosity, gas-phase tortuosity, water-vapor diffusivity

Fixed Secondary Variables: aqueous-phase viscosity

Fluxes: aqueous-phase velocity, gas-phase velocity, water-vapor diffusion mass flux

2.4.4 Energy

Description: The Energy mode solves heat transfer problems for saturated and unsaturated subsurface flow problems. Constant aqueous- and gas-phase flow fields may be prescribed. Diffusive heat transfer occurs through the solid and liquid phases. Advective heat transfer occurs through the fluid phases. No heat transfer occurs by vapor diffusion through the gas phase. System pressures, phase saturations, and relative permeabilities are invariant. Mass continuity is not ensured for specified flow fields. Physical properties may be specified as invariant or temperature dependent.

Application: Appropriate applications for the Energy mode include subsurface heat transfer through saturated and unsaturated porous media. Fixed saturation and fluid flow fields are the principal assumptions associated with this mode. Saturation levels and Darcy flow velocities may be specified for the aqueous and gas phases through the initial pressure fields and soil characteristics. An appropriate application for this mode could involve heat transfer through completely dry or completely saturated porous media, or heat transfer through partially saturated porous media with relatively high liquid mass flux rates. Without adjusting the porous media thermal conductance for heat transfer enhancement by vapor diffusion, this mode would be inappropriate for predicting heat transfer for partially saturated media with low liquid mass flux rates. The mode would also be inappropriate for conditions where the thermal field affected the saturation fields (e.g., heat-pipe flow phenomena).

Specification: Solution Schemes card

- Governing Equations
  - Thermal Energy Conservation Equation: on
  - Water Conservation Equation: off
  - Air Conservation Equation: off
  - Species Conservation Equation: off
- Options
  - Binary Diffusion: off
  - Fixed Properties: off / on
  - Liquid Phase: off / on
  - Gas Phase: off / on
  - Vapor Pressure Lowering: off

Primary Variables: temperature

Fixed Primary Variables: aqueous pressure, gas pressure

Secondary Variables: water-vapor partial pressure, air partial pressure, water-vapor density, air density, gas-phase density, aqueous-phase density, water-vapor mass/mole fraction, air mass/mole fraction, aqueous-phase air mass fraction, water-vapor enthalpy, air enthalpy, gas-phase enthalpy, aqueous-phase enthalpy, water-vapor internal energy, air internal energy, gas-phase internal energy, aqueous-phase internal energy, aqueous-phase thermal conductivity, solid-phase thermal conductivity, equivalent thermal conductivity

Fixed Secondary Variables: aqueous-phase saturation

Fluxes: thermal flux

2.4.5 Water-Energy

Description: The Water-Energy mode solves aqueous flow and heat transfer problems for saturated and unsaturated subsurface flow systems. Aqueous-phase flow fields are computed assuming a nonparticipating gas phase. Soil characteristics are computed for an air-water system using nonhysteretic relations. Diffusive heat transfer occurs through the solid and aqueous phases. Advective heat transfer occurs through the aqueous phase. No heat transfer occurs by vapor diffusion through the gas phase. Physical properties may be specified invariant or dependent on aqueous pressure and temperature. Species transport in the aqueous phase may be modeled by additionally solving the species mass conservation equation.

Application: Appropriate applications for the Water-Energy mode include ground-water flow and heat transfer through saturated and unsaturated porous media. Typical applications would involve concurrent solutions of the aqueous pressure and temperature fields. Transport of heat and water vapor through the gas phase is assumed negligible with this mode. An appropriate application for this mode could be the solution of a density-driven aqueous flow through porous media. Inappropriate problems include those characterized with high latent heat transfer rates through the gas phase.

Specification: Solution Schemes card

- Governing Equations
  - Thermal Energy Conservation Equation: on
  - Water Conservation Equation: on
  - Air Conservation Equation: off
  - Species Conservation Equation: off / on
- Options
  - Binary Diffusion: off
  - Fixed Properties: off / on
  - Liquid Phase: on
  - Gas Phase: off / on
  - Vapor Pressure Lowering: off

Primary Variables: aqueous pressure, temperature

Fixed Primary Variables: gas pressure

Secondary Variables: aqueous-phase density, aqueous-phase viscosity, aqueous-phase enthalpy, aqueous-phase internal energy, aqueous-phase thermal conductivity, solid-phase thermal conductivity, equivalent thermal conductivity, aqueous-phase saturation, trapped gas saturation, aqueous-phase relative permeability, porosity, aqueous-phase tortuosity

Fluxes: aqueous-phase velocity, thermal flux

2.4.6 Air-Energy

Description: The Air-Energy mode solves unsaturated subsurface gas flow and heat transfer problems with static saturation fields. Liquid saturations are temporally invariant, and are either specified or computed from initial fields of aqueous pressure and gas pressure. Diffusive heat transfer occurs through the solid and liquid phases. Advective heat transfer occurs through the gas phase. No heat transfer occurs by vapor diffusion through the gas phase. Conservation of water mass is not ensured for vapor transport problems. Physical properties may be specified invariant or dependent on gas pressure and temperature. Species transport in the gas phase may be modeled by additionally solving the species mass conservation equation.

Application: Appropriate applications for the Air-Energy mode include gas flow and heat transfer through unsaturated porous media. Density-driven gas flows resulting from transient or steady thermal fields would be an appropriate problem for this mode. Fixed liquid saturation fields may be specified for the aqueous phase through the initial aqueous and gas pressure fields and the soil characteristics. For these types of applications, the influence of both temperature and vapor mass fractions on gas-phase properties could be investigated. An inappropriate application, however, would result if the liquid saturation fields were significantly altered by the transport of vapor or heat through the gas phase.

Specification: Solution Schemes card

- Governing Equations
  - Thermal Energy Conservation Equation: on
  - Water Conservation Equation: off
  - Air Conservation Equation: on
  - Species Conservation Equation: off / on
- Options
  - Binary Diffusion: off / on
  - Fixed Properties: off / on
  - Liquid Phase: off
  - Gas Phase: on
  - Vapor Pressure Lowering: off / on

Primary Variables: gas pressure, temperature

Fixed Primary Variables: aqueous pressure

Secondary Variables: water-vapor partial pressure, air partial pressure, water-vapor density, air density, gas-phase density, water-vapor mass/mole fraction, air mass/mole fraction, gas-phase viscosity, water-vapor enthalpy, air enthalpy, gas-phase enthalpy, aqueous-phase enthalpy, water-vapor internal energy, air internal energy, gas-phase internal energy, aqueous-phase internal energy, aqueous-phase thermal conductivity, solid-phase thermal conductivity, equivalent thermal conductivity, water-vapor diffusivity

Fixed Secondary Variables: aqueous-phase saturation

Fluxes: gas-phase velocity, water-vapor diffusion mass flux, thermal flux

2.4.7 Water-Air-Energy

Description: The Water-Air-Energy mode solves aqueous flow and heat transfer problems for saturated and unsaturated subsurface flow systems. Aqueous-phase flow fields are computed assuming a participating gas phase. Soil characteristics are computed for an air-water system using nonhysteretic relations. Diffusive heat transfer occurs through the solid and aqueous phases. Advective heat transfer occurs through the aqueous and gas phases. Diffusive heat transfer through the gas phase includes both sensible and latent components for water vapor. No heat transfer occurs by vapor diffusion through the gas phase. Physical properties may be specified invariant or dependent on aqueous pressure, gas pressure, and temperature. Species transport in the aqueous and gas phases can be modeled by additionally solving the species mass conservation equation.

Application: Appropriate applications for the Water-Air-Energy mode include aqueous and gas flow and heat transfer through saturated and unsaturated porous media. Because of the coupled solution of the water, air, and energy equations, this mode is applicable to problems involving both sensible and latent heat transfer through the gas phase (e.g., heat-pipe flow). This mode eliminates the isothermal assumptions associated with the Water-Air mode and the assumptions of zero latent heat transfer associated with the Water-Energy mode, at a cost of additional computational effort.

Specification: Solution Schemes card

- Governing Equations
  - Thermal Energy Conservation Equation: on
  - Water Conservation Equation: on
  - Air Conservation Equation: on
  - Species Conservation Equation: off / on
- Options
  - Binary Diffusion: off / on
  - Fixed Properties: off / on
  - Liquid Phase: on
  - Gas Phase: on
  - Vapor Pressure Lowering: off / on

Primary Variables: aqueous pressure (water-vapor mass fraction), gas pressure, temperature

Secondary Variables: water-vapor partial pressure, air partial pressure, water-vapor density, air density, gas-phase density, aqueous-phase density, air mass/mole fraction, water-vapor mass/mole fraction, aqueous-phase air mass/mole fraction, gas-phase viscosity, aqueous-phase viscosity, water-vapor enthalpy, air enthalpy, gas-phase enthalpy, aqueous-phase enthalpy, water-vapor internal energy, air internal energy, gas-phase internal energy, aqueous-phase internal energy, aqueous-phase thermal conductivity, solid-phase thermal conductivity, equivalent thermal conductivity, aqueous-phase saturation, gas-phase saturation, trapped gas saturation, aqueous-phase relative permeability, gas-phase relative permeability, porosity, aqueous-phase tortuosity, gas-phase tortuosity, water-vapor diffusivity

Fluxes: aqueous-phase velocity, gas-phase velocity, water-vapor diffusion mass flux, thermal flux

3.0 Graphical Input Overview

The MSTS Graphical Input is an independent application that provides a relatively easy way to prepare MSTS input files. The traditional way to prepare simulation input/control files for numerical simulators is to use a text editor and type in the necessary information following the format required by the particular simulation code to be used. This is still possible with the MSTS code, but the MSTS Graphical Input provides an alternative point-and-click method that simplifies input file preparation.

The MSTS Graphical Input has three functions: 1) to prepare MSTS input files, 2) to perform a few elementary consistency checks on these files, and 3) to compute the minimum size of certain MSTS code parameters for a particular input file. The input file written by MSTS Graphical Input is an ASCII text file that exactly meets the input file format requirements of the MSTS code. This format is given in detail in Section 6.0 (Input File Structure).

The MSTS Graphical Input includes another feature to enhance its usefulness; online, context-sensitive help is available at any time the Graphical Input is in use. To activate this feature, press ⌘H (command and H keys together) or select Help from the Window menu. The help window that appears will contain information on the input card that is currently open. Information on other subjects is available by selecting topics from the main Help menu or by searching on keywords. Close the help window when finished to return to the input card last active.

For a complete introduction to the use of the MSTS Graphical Input, refer to Section 5.0 (MSTS Quick Tour). The Quick Tour will guide you through a small, but complete, numerical simulation of vertical water infiltration to demonstrate the use of the MSTS Graphical Input and the MSTS computer code.

4.0 File Management

MSTS input/output and source code file management is relatively straightforward and simple. This section is not highly specific about file management because MSTS can be used on such a variety of platforms (e.g., Macintosh, Cray, Sun, Convex, and HP). Instead, a few general guidelines common to the use of MSTS on any computing platform are provided. It is the responsibility of the users to adapt these guidelines to their particular computer platforms and operating systems.

4.1 MSTS Input and Output Files

All input and output files used by the MSTS code are listed in Table 4.1 with a brief description of the function or contents of each. All input and simulation control is accomplished using the "input" file, whereas output is directed to several of the files named in Table 4.1. This "input" file may be prepared either with a text editor or by using the MSTS Graphical Input. The Graphical Input is described in Section 3.0, and a detailed reference of the input file format is provided in Section 6.0. The MSTS code always searches for the file names listed in Table 4.1 in the default directory during execution.

If an output file already exists in the default directory with the same file name as one MSTS must use, it will overwrite the existing file. Therefore, to keep copies of output files from previous simulations, the user must either 1) maintain all input and output files associated with a single simulation in a separate directory or 2) rename the input and output files that are to be kept with file names that do not appear in Table 4.1. In the first approach, the user typically would give the directory a name descriptive of the simulation (e.g., "sim1" or "run03"). In the second approach, the user should give file names that group the simulation together, such as renaming the "output," "surface," and "debug" files to "run01.out," "run01.srf," and "run01.dbg," respectively.

The restart file requires special attention. If a simulation requires a restart file, the file must be in the default directory and must be named "restart". Be cautious, however; MSTS will read the existing restart file, perform the simulation, and then overwrite the restart file with the conditions at the end of the new simulation. Hence, to keep a copy of the original restart file, which is recommended in case the restarted simulation must be repeated for any reason, the user should make a copy of the restart file prior to using it. If using a separate directory for each simulation, simply copy the restart file to the directory intended for the new simulation. If renaming files by

Table 4.1. MSTS Input and Output File Name Convention

File Name	Type[a]	Contents
input	i	parameter input and simulation control commands
output	o	echo of simulation input, simulation progress, and selected field variable output
restart	io	values of field variables in model domain at end of simulation
surface	o	surface flux integrator output
debug	o	optional debugging information

(a) i = input file (read by MSTS)
o = output file (written by MSTS)
io = both input and output (written by MSTS for later use)

simulation, copy the restart file (rather than renaming it) to some non-MSTS file name (e.g., "run01.res").

4.2 MSTS Source Code Parameterization

The MSTS source code file, "msts.f," is a text file that contains approximately 20,000 lines of source code and comments written in FORTRAN 77, following the American National Standards Institute (ANSI) standards. A user must usually make two general modifications to the source code before executing the code: parameterization and machine specification (discussed in Section 4.3). Parameterization involves modifying the parameter statements in the source code to fit a particular class of problems. This section presumes that users are familiar with the operating systems and text editors for their computing environments.

To parameterize a code, first determine the size of each parameter. Table 4.2 provides a list of MSTS parameters and their functions and computations. The computations provided in Table 4.2 give the minimum size of each parameter; these can be larger, but larger parameters will increase the size of the executable file. It is usually best to compute the largest value of each parameter for all simulations of a particular problem you wish to run and parameterize the MSTS code with those values. Once you have determined the parameter values, use a text editor to open the MSTS source code file and navigate to the first parameter statement block (usually within the first 50 lines of source code); it will look like this:

Table 4.2. MSTS Parameters

Parameter	Description
LFX	maximum number of x- or r-nodes
LFY	maximum number of y- or θ-nodes
LFZ	maximum number of z-nodes
LFLD	maximum number of nodes (LFLD=LFX*LFY*LFZ)
LROW	Minimum value of LROW depends on the solution scheme chosen. For any method, ISLVS is the number of coupled equations that will be solved and ranges from 1 to 3 (add 1 each for thermal energy, water mass, and air mass conservation equations; species mass is not a coupled equation and does not affect ISLVS). Banded Matrix: Compute IJFLD = LFX * LFY Compute JKFLD = LFY * LFZ Compute KIFLD = LFX * LFZ If IJFLD ≤ JKFLD and IJFLD ≤ KIFLD, then LROW = 3 * (ISLVS * IJFLD + ISLVS - 1) + 2 Else if JKFLD ≤ KIFLD and JKFLD ≤ IJFLD then LROW = 3 * (ISLVS * JKFLD + ISLVS - 1) + 2 Else if KIFLD ≤ IJFLD and KIFLD ≤ JKFLD then LROW = 3 * (ISLVS * KIFLD + ISLVS - 1) + 2 Conjugate Gradient: ROW = ISLVS * LFLD + 1
LCOUP	(LFLD - NPX) * ISLVS + 1, where NPX is the total number of inactive nodes
LZN	maximum number of rock or soil type declarations
LSN	maximum number of source term declarations
LBC	maximum number of boundary node conditions declared for any one boundary condition card (maximum number of nodes with specified boundary conditions in liquid boundary, gas boundary, vapor boundary, thermal energy boundary, or species boundary condition cards).
LST	maximum number of entries in <u>all</u> source term tables together
LSCT	maximum number of rock or soil characteristic declarations
LRPT	maximum number of relative-permeability declarations
LSF	maximum number of surface flux integrator declarations
LCHR	maximum number of characters in any input card (usually set to 1000 for convenience)

```
C-----------------------------------------------------------------------C
C     Parameter Statements.
C-----------------------------------------------------------------------C
      PARAMETER( LFX=91, LFY=1, LFZ=50, LX=LFX+2, LY=LFY+2, LZ=LFZ+2 )
      PARAMETER( LFLD=4550, LROW=458, LCOUP=13651, LZN=7, LSN=11 )
      PARAMETER( LBC=728, LST=634, LSCT=1, LRPT=12, LSF=25, LCHR=1000 )
      PARAMETER( LSX=((LFX+1)*LFY*LFZ), LSY=(LFX*(LFY+1)*LFZ) )
      PARAMETER( LSZ=(LFX*LFY*(LFZ+1)) )
```

Only the first three statements are ever changed; the last two (LSX, LSY and LSZ) never require modification. These parameter statements appear in exactly this form in dozens of places in the source code; the easiest way to change them is to prepare a block of text that replaces the first three lines and use the search-and-replace feature common to most text editors. For example, if we wish to change the parameter statements shown above so that LFY is increased to 5 and the number of rock or soil types (parameter LZN) is increased to 9, then we begin by making a copy of the three lines of parameter statements and making the desired changes to the copy:

```
      PARAMETER( LFX=91, LFY=5, LFZ=50, LX=LFX+2, LY=LFY+2, LZ=LFZ+2 )
      PARAMETER( LFLD=4550, LROW=458, LCOUP=13651, LZN=9, LSN=11 )
      PARAMETER( LBC=728, LST=634, LSCT=1, LRPT=12, LSF=25, LCHR=1000 )
```

Next, order the text editor to search for occurrences of those original three lines in the file and to replace them with the three new lines. When all occurrences are replaced with the new lines, save the newly parameterized source code file to your working directory (do not overwrite your original source code!).

A time-saving feature of the MSTS Graphical Input is the "Compute Parameters" feature. Once you have finished preparing an input file and have saved it, choose the "Compute Parameters" feature and select the input file of interest. The Graphical Input will compute the minimum required parameters for that input file and display them on screen; more useful yet, it will write the three parameter statements to a file entitled "parameters" in the default directory. Now all you have to do to parameterize the code is open the MSTS source code file and the parameter file with your text editor and use the contents of the parameter file as the text to replace the old parameter statements.

4.3 MSTS Source Code Machine Specification

Machine specification involves changing certain commented lines in the MSTS source code into executable statements so that the code is customized for a particular computer. Ordinarily, these lines of code are concerned with obtaining the execuation time and date from the host computer for quality assurance purposes. Because the way in which the computer's clock is accessed is different from one computer to the next, some machine-specific code is necessary.

Such code has been included for a number of machines in the "msts.f" file, and then "commented-out" so that none of the machine-specific code is active is the distribution "msts.f" file. A special "comment block" name has been reserved for each computer supported by the MSTS code, such as "CMAC" for Macintosh. Here is an example of Macintosh-specific code in MSTS:

```
C-----------------------------------------------------------------------C
C     Macintosh Environment.
C-----------------------------------------------------------------------C
CMAC      ISC = 9
```

To make the code ready to compile on the Macintosh, remove the "CMAC" comment block:

```
C-----------------------------------------------------------------------C
C     Macintosh Environment.
C-----------------------------------------------------------------------C
         ISC = 9
```

This must be done for all occurences of "CMAC" in the code. The efficient way to do this is to use the search-and-replace feature of your text processor to find all occurences of "CMAC" (or the appropriate comment block for your machine) and replace it with four spaces.

Table 4.3 lists the machines and associated comment block names that were available in the "msts.f" file at the time this document was written. Other machines may have been added since, so check the source code file if your machine does not appear in Table 4.3.

Table 4.3. MSTS-Supported Machines and Associated Comment Blocks

Computer	Comment Block Name
Apple Macintosh	CMAC
Sun	CSUN
IBM (AIX)	CIBM
Stellar	CSTLR
HP 9000	CHP
Convex	CNVX
Cray	CRAY

5.0 MSTS Quick Tour

This section leads the new MSTS user through a quick tour of both use of the MSTS Graphical Input and an application of the MSTS code. Following the tour outlined in this section is highly recommended for new MSTS users as a fast way to "come up to speed" on the use of MSTS. The quick tour leads the reader through the steps necessary to create an input file for performing a one-dimensional simulation of vertical water infiltration into a generic sand. This section assumes that the reader is using a Macintosh computer with a FORTRAN compiler installed and has a basic mastery of the Macintosh computing environment. Terms such as "point and click," "double-click," "drag," and "launch" should be familiar to the reader. It is further assumed that the user understands the fundamentals of unsaturated flow in porous media that are simulated in this tour. The quick tour requires approximately 2 hours to complete.

5.1 Installing MSTS on a Macintosh Computer

If not already done, install the MSTS source code and the MSTS Graphical Input application on your Macintosh's hard disk. Insert the distribution disk containing the MSTS source code into the floppy disk drive and drag the "msts.f" icon to an appropriate folder in your hard disk. After the file is copied, eject the floppy disk and insert the disk containing the MSTS Graphical Input application. Copy this file to the same folder you put the source code in and eject the second disk.

5.2 Launching the MSTS Graphical Input

Launch the MSTS Graphical Input either from the menu (select the icon, then choose Open from the File menu) or by double-clicking the application icon. The MSTS Graphical Input information window (Figure 5.1) will be displayed while the application loads. A new menu bar (Figure 5.2) replaces the Macintosh Finder menu when the Graphical Input is loaded. The menu bar includes the familiar Apple, File, and Edit menu items, plus several menu items that are unique to the Graphical Input menu bar.

5.3 Creating a New Input File

To create a new simulation file, select New from the File menu. Specify the input file name and folder using the dialog box (Figure 5.3) that appears next. Enter the name "input" in the box titled "New Input Title" and choose a folder. Click the Save button to continue. When creating a

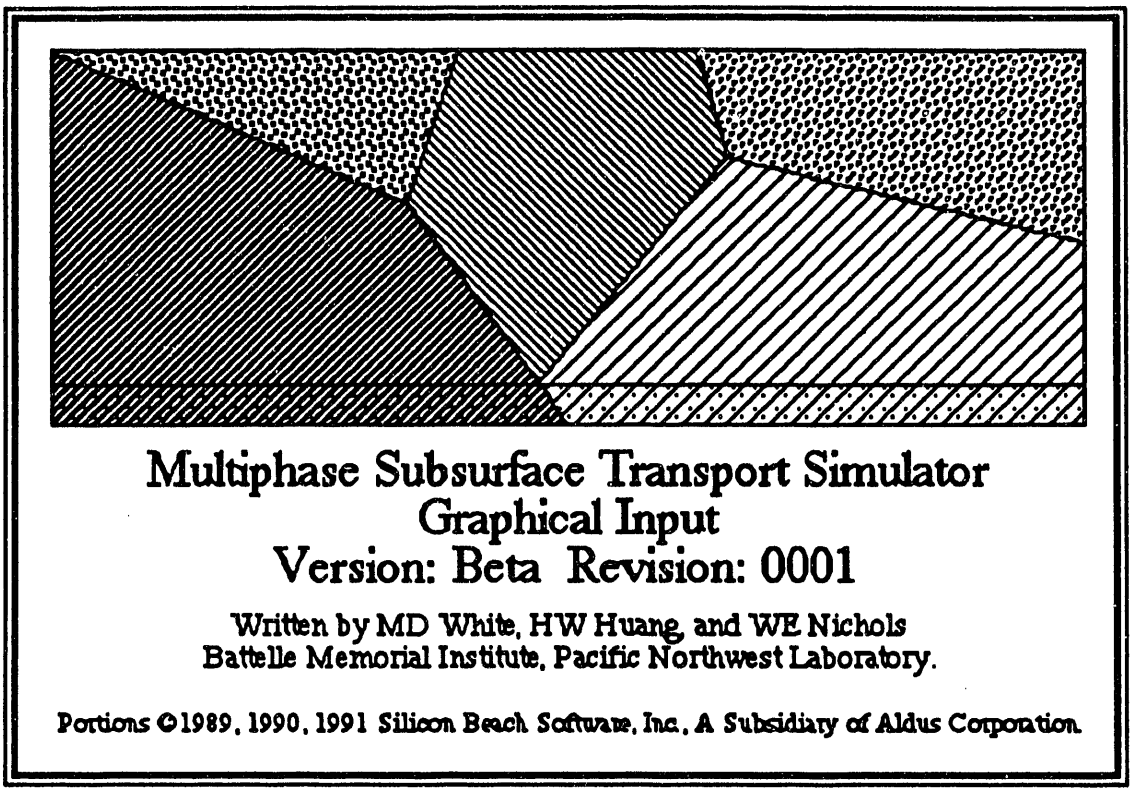

Figure 5.1. Information Window from MSTS Graphical Input

Figure 5.2. Menu Bar from MSTS Graphical Input

new input file, the Graphical Input responds with a dialog box that asks if you wish to initialize all cards (Figure 5.4). If the Yes button is selected, all data-entry fields will be initialized to blank fields or default values. Otherwise, all data fields will contain the data entered most recently since the last initialization (including previous Graphical Input sessions). Individual cards may be initialized by selecting the Initialize item from the File menu while the card is open. Click on the Yes button. A feature of the Graphical Input is the ability to hold the most recent options and user entries in memory until replaced or initialized. This feature can be useful if you are preparing a new input file that is only slightly different from the last one you prepared, and saves recalling the old file before modifying it. To begin with a clean slate, though, initialize all cards.

Next, the Main Menu card will appear, centered on your screen (Figure 5.5). This card will have the input file name on the window bar (top) and two columns of labeled buttons. Each button

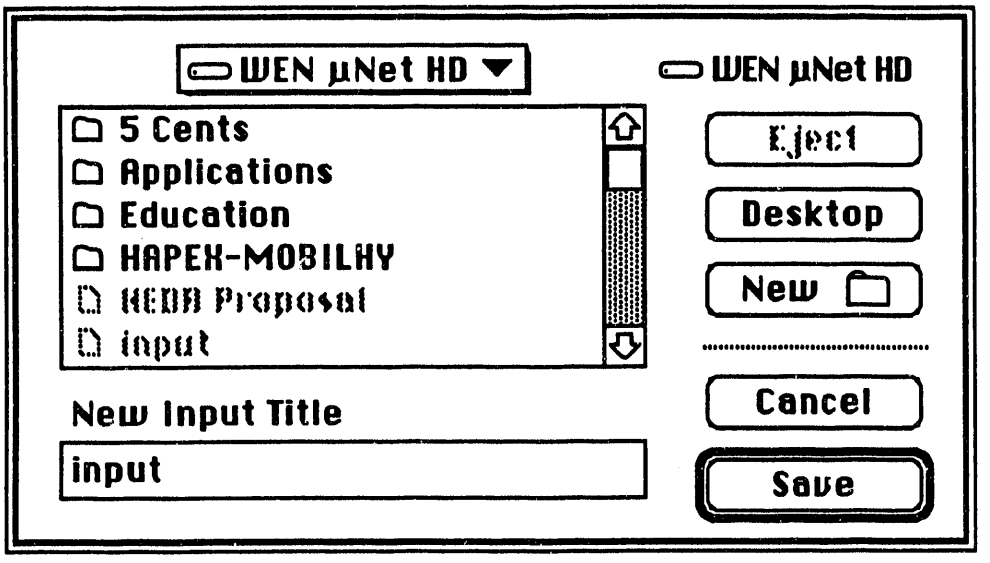

Figure 5.3. File Dialog Box from MSTS Graphical Input

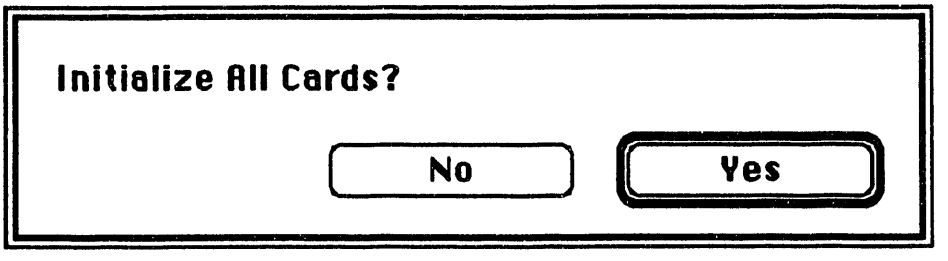

Figure 5.4. Initialization Prompt for New Input Files

corresponds to a particular MSTS input card and when clicked, opens that card. We will begin preparing the simulation input file with the Simulation Title card. Click on the top button of the left column of buttons, labeled "Simulation Title." The card that appears (Figure 5.6) is used to enter record information (e.g., simulation title, user's name and affiliation, file creation date, and notes about the simulation). Complete these fields with your own personal information, using Figure 5.6 as a guide. Clicking the Date button will automatically enter the file creation date and time.

5.4 Navigating Between Input Cards

The four arrow icons at the top right of the input card (Figure 5.6) allow you to navigate between input cards. When clicked, the first arrow will always return you to the Main Menu card; the second arrow (pointing left) will open the previous input card in the input card order (that is,

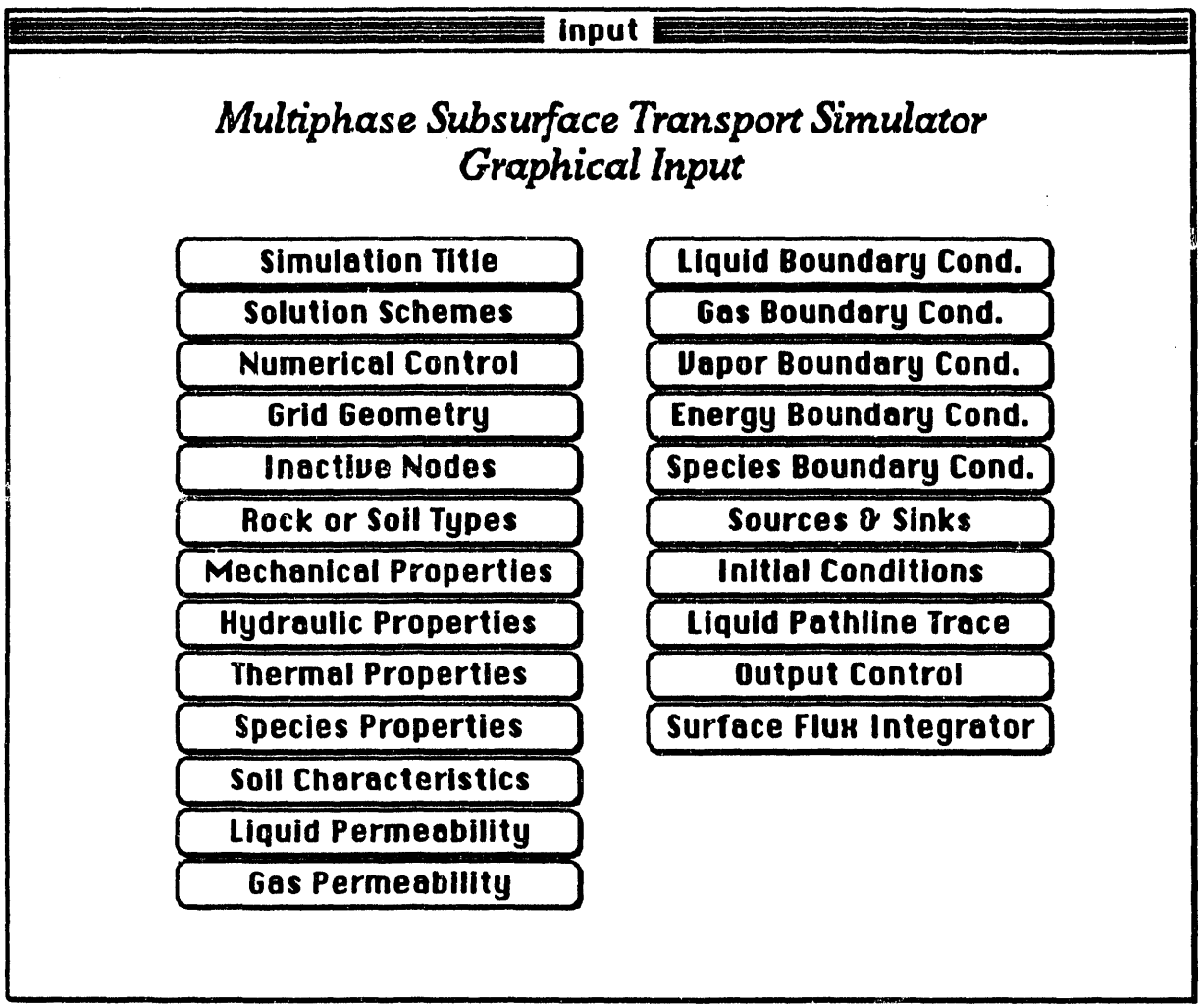

Figure 5.5. Main Menu Card from MSTS Graphical Input

the order in which the cards appear in Table 6.1 of Section 6.0, and in the MSTS "input" file); the third arrow (pointing right) will call the next input card in the input card order; and while the last arrow will open the next-higher-level card returning up the hierarchy of card levels. Click the last arrow to return to the Main Menu card. Reading down the left column of buttons on the Main Menu card, the next button after Simulation Title is Solution Schemes; click on the Solution Schemes button to navigate to that input card.

5.4.1 Solution Schemes

The Solution Schemes input card (Figure 5.7) allows you to specify the solution options, the simulation time period, the solution technique, and other control information. Click on the Water

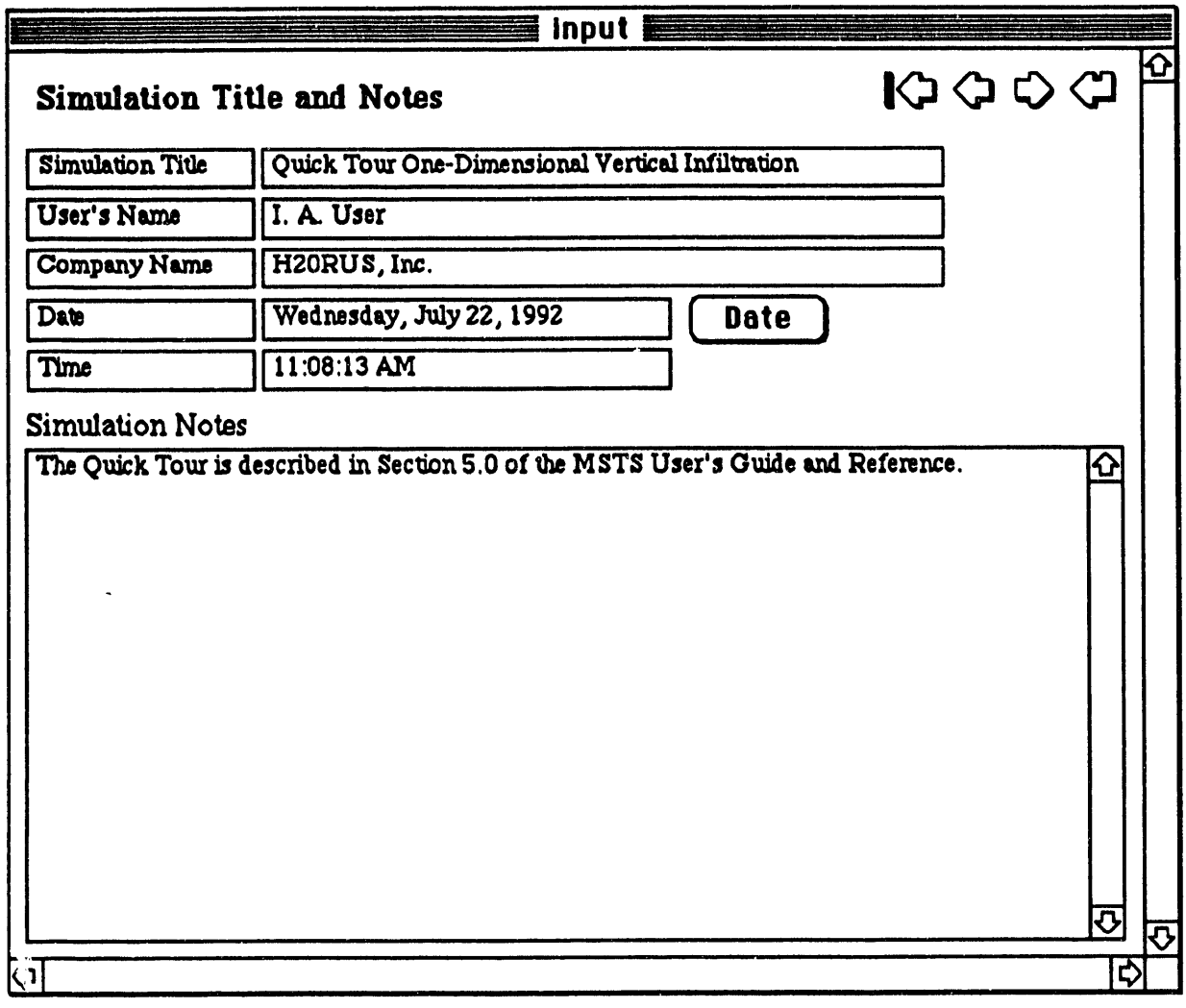

Figure 5.6. Simulation Title Input Card Example

Conservation box (but not the other three, Thermal Energy, Air Conservation, or Species Concentration) to invoke the Water mode (see Section 2.4 for more information on solution methods available). To fill the data arrays in MSTS and examine initial conditions without solving the equations, check the Initial Conditions Only box. The initial conditions option is useful for computing saturations and physical properties from the initial primary variables specified either in the Initial Conditions card or in a restart file. We will avoid that option for now. Because we are starting from the beginning, leave the Restart box unchecked.

To enter the solution limits information, click on the Units button, drag down the button menu, and select "h" (hours). Enter in the respective boxes a time limit of 2.0 hours, an initial

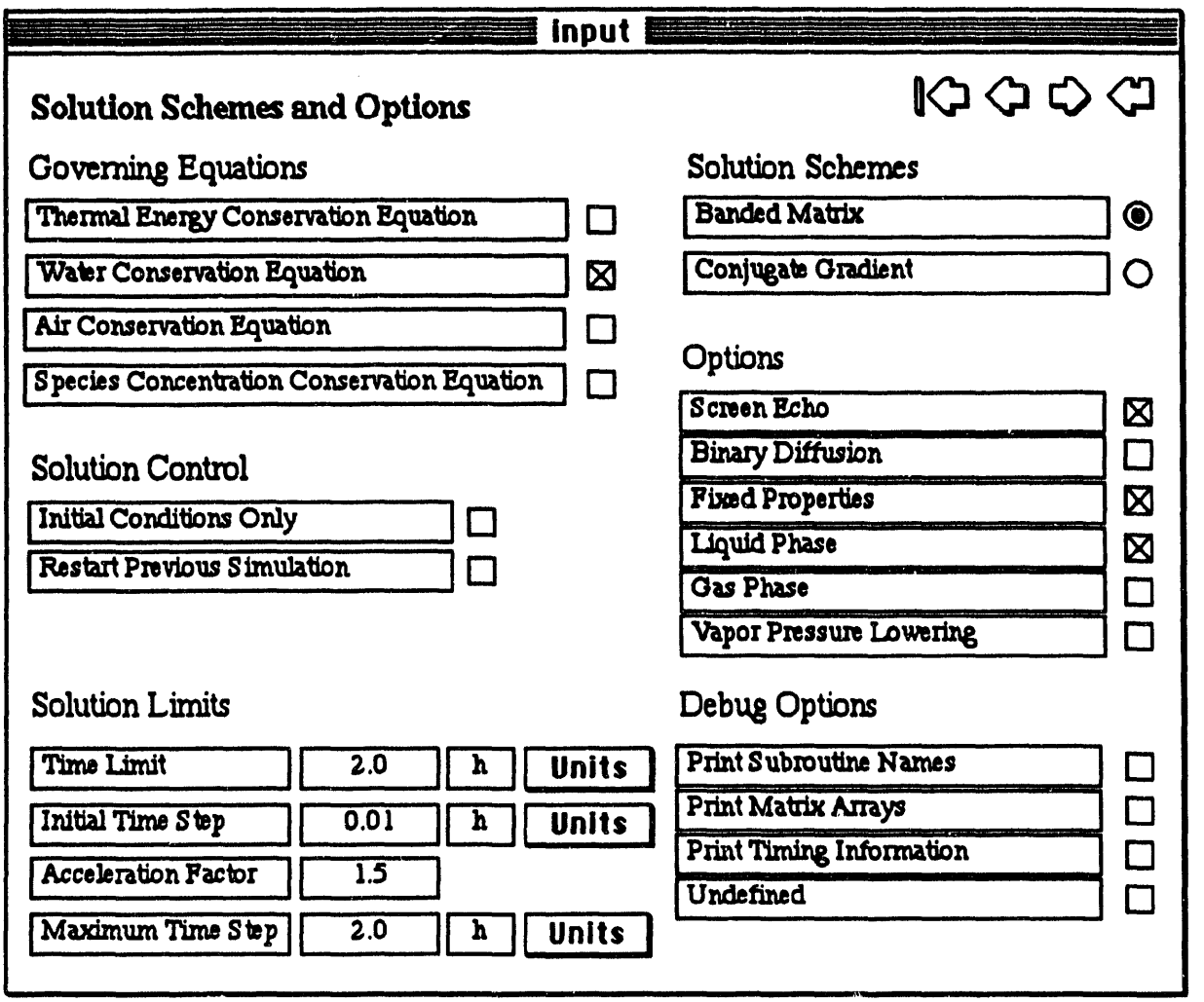

Figure 5.7. Solution Schemes Input Card Example

time step of 0.01 hour, a time-step acceleration factor of 1.5, and a maximum time step of 2.0 hours. These numbers control, respectively, the time length, the initial time step, the acceleration factor that specifies how fast MSTS will try to increase the time step (a factor of 1.5 would mean a 1-second time step would be increased to 1.5 seconds on the second step, 2.25 seconds on the third step, and so on until a convergence limit is exceeded), and the maximum time step. Because we chose hours as the time unit, all solution limits are expressed in units of "h".

Under "Solution Schemes," check the Banded Matrix option. This is usually acceptable for most simulations. Refer to Section 4.6 of the MSTS Theory Manual (White and Nichols 1992) for a discussion of the available linear-equation solution schemes.

"Options" include an assortment of check boxes. Check the Screen Echo box so that MSTS will report reference node information to your computer screen during the simulation execution. Also check the Fixed Properties box, which is used to prevent MSTS from recomputing certain physical properties (e.g., fluid density) each time step, thus achieving a faster execution for problems where these properties do not vary. The Fixed Properties option should not be invoked for problems involving variable physical properties (e.g., density-driven flow through porous media). The Liquid Phase box was automatically checked for you when you activated the water conservation governing equation; leave this box checked. Because we are not considering gas-phase migration of water vapor, do not check the Gas Phase box. Do not check any of the "Debug Options" either; these are not needed for our quick tour.

5.4.2 Numerical Control

Click the third arrow at the top right-hand corner of the Solution Schemes input card to navigate to the Numerical Control card. Enter 8 in the Maximum Iterations per Step field. This number limits the number of Newton-Raphson iterations per convergence attempt. Select the Maximum Residual convergence mode from the next button. Set the "CPU Limit" and "Wallclock Limit" to 1 hour each (remember to set the time units to hours with the Units buttons). Finally, set the convergence criteria to 1.0×10^{-6} (enter this as 1.0E-06) for the water equation and choose the Geometric Mean option for property averaging for the water equation. The case of the "e" exponent indicator is unimportant for MSTS input, as are leading zeros (e.g., 1.0E-06 is the same as 1.e-6). Convergence criteria and averaging techniques may be set for the other equations as well but are not needed because only the water conservation equation will be solved. Navigate to the next card (Grid Geometry).

5.4.3 Grid Geometry

The quick tour problem requires a one-dimensional, vertical model domain. Begin constructing the grid by checking that the coordinate system is Cartesian; if the radio button next to the "Cylindrical Grid" on the right side of the Grid Geometry input card (Figure 5.8) is highlighted, check "Cartesian Grid" instead. Enter numbers in the fields under the "Number of Nodes" portion of the input card so that there is 1 node in the x-direction, 1 node in the y-direction, and 20 nodes in the z-direction. Then indicate for "Grid Dimensions" that the x- and y-dimensions are 1 cm, and the z-dimension is 20 cm. The datum elevation and the grid bottom elevation should both be 0 cm. At this point we could enter the node positions manually, by entering the values and accepting them, but a faster way to construct the grid for uniformly spaced nodes is to click the Uniform button. The Graphical Input will generate the node coordinates and record them in the

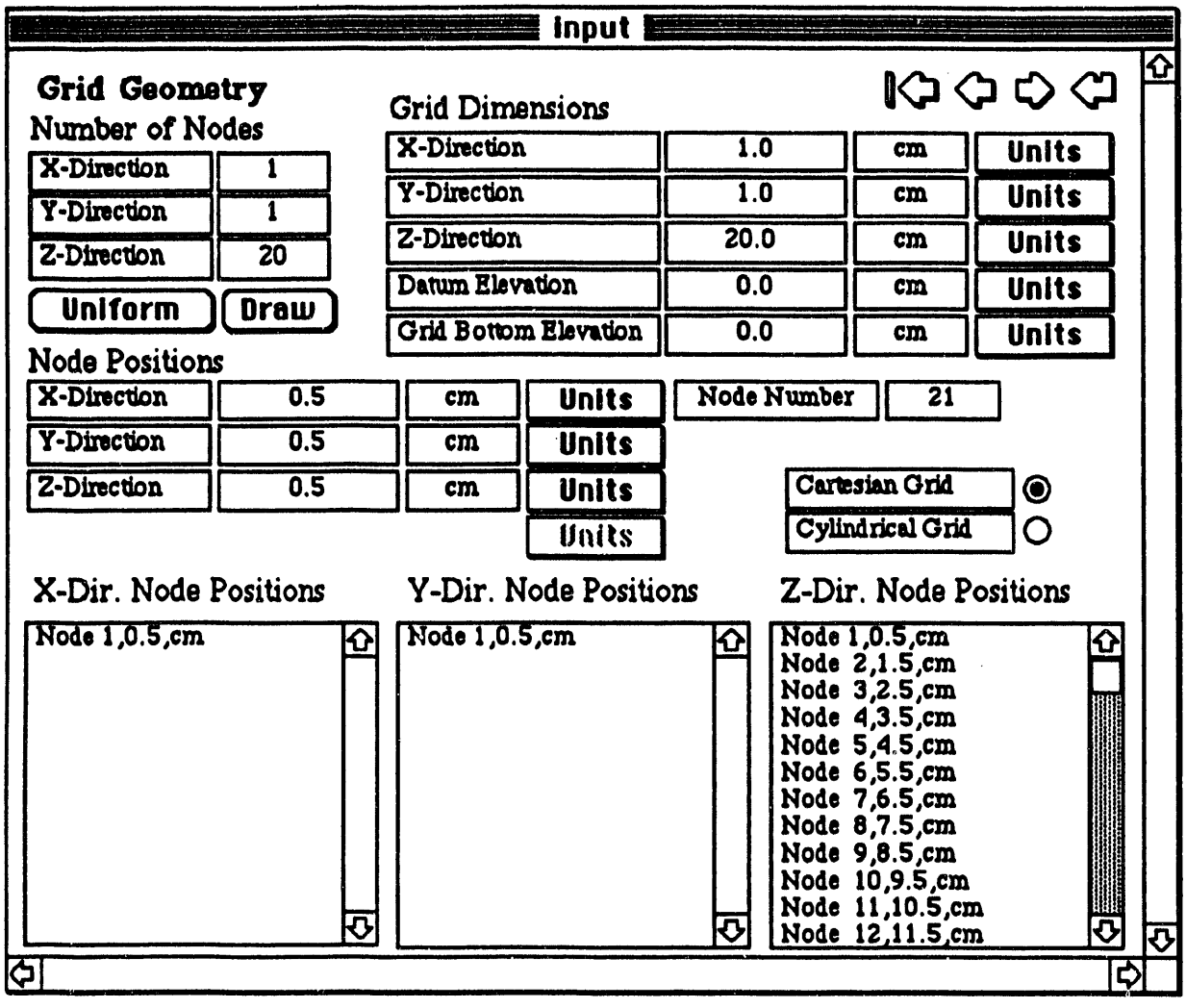

Figure 5.8. Grid Geometry Input Card Example

appropriate fields at the bottom of the Grid Geometry card (see Figure 5.8). There are no inactive nodes in this problem, so navigate to the Rock or Soil Types card.

5.4.4 Rock or Soil Types

Our simulation domain comprises only one type of porous material, which we term generic sand. Click in the blank field next to the box titled "Rock Name" and type "Generic Sand" to identify the soil. If this medium filled only a portion of the domain, we would enter the node number ranges in x, y, and z to indicate its extent. Because the generic sand extends over the whole domain, we simply click the Entire Domain button to have the Graphical Input automatically fill these fields with the maximum node range. Note that use of the Entire Domain button requires that

the Grid Geometry card already be completed. Now the soil type is specified but not recorded; press ⌘A (command and A keys together) or select Accept from the Edit menu to record the rock or soil type in the Rock List (more about that later). After the entry is recorded, a line will appear in the scrolling box at the bottom of the card that looks like this:

```
Generic Sand,1,1,1,1,1,20,
```

Navigate to the next card (Mechanical Properties).

5.4.5 Mechanical Properties

Choose Rock List from the Windows menu. A floating window will appear (Figure 5.9) that contains the names of all rock types you have recorded. At this point, only one name will appear: "Generic Sand." If you double-click on "Generic Sand" in the Rock List, the name will be placed in the Rock Type field of the Mechanical Properties card (or any other input card with a field entry titled "Rock name"). You may use the Rock List to pick rock or soil types for any card that requires one. Close the Rock List. Enter total porosity of 0.40, diffusive porosity of 0.50, and effective porosity of 0.30. Ignore the tortuosity option fields; these are unnecessary for this tour. Now accept the entry (press ⌘A or select Accept from the menu). Have you noticed the authors' mistake yet? Diffusive porosity cannot exceed total porosity; we have reversed these numbers, so the two must be corrected. This may be done in two ways. One is to select the record line that was to be corrected (click once on the line and it will highlight), and delete it by pressing ⌘D or selecting Delete from the Edit menu. Then correct the entry and accept it again. The other way is to replace the record line by correcting the Total Porosity and Diffusive Porosity fields, then highlight the line and press ⌘R (or choose Replace from the Edit menu with the line highlighted). Using either method, correct the porosity entries for generic sand. The Accept, Delete, and Replace functions are similar for all input cards in the Graphical Input. Navigate to the next card (Hydraulic Properties).

5.4.6 Hydraulic Properties

By now you should be able to see the pattern for input card preparation. Test your ability by picking the rock type and entering a *z*-direction hydraulic conductivity of 1.0×10^{-2} cm/s (enter as 1.0E-02). Porous media transmissivity may be expressed with either a hydraulic conductivity at 20°C or an intrinsic permeability. Units preceded by "hc:" are for hydraulic conductivity and are expressed as length per time ($L\ t^{-1}$), whereas intrinsic permeability units are measured in length squared (L^2). Accept your entry and navigate to the Soil Characteristics card (we will skip the

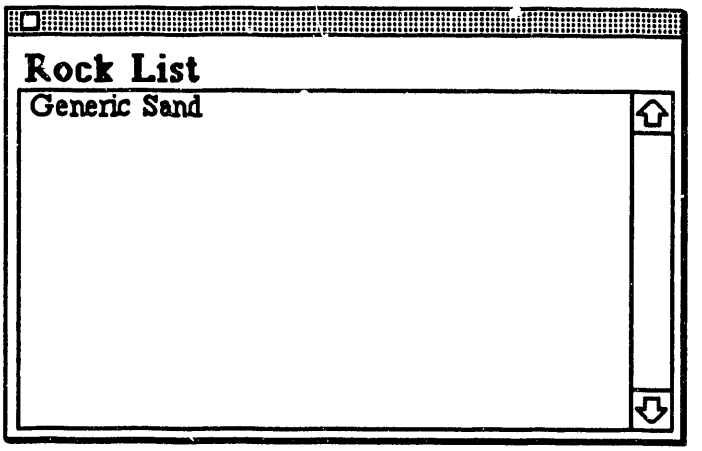

Figure 5.9. Rock List from MSTS Graphical Input

Thermal Properties and Species Properties cards because the quick tour problem is not concerned with heat transfer or species transport).

5.4.7 Soil Characteristics

Select Generic Sand from the Rock List and choose van Genuchten from the Moisture Retention button menu. Enter an α (alpha) parameter value of 0.05 1/m, an n parameter value of 1.5, and a maximum tension head value of 1.0×10^5 m (1.0E+5). The online help feature of the Graphical Input may be used to inquire about the van Genuchten function. To invoke this feature, press [⌘][R] or choose Help from the Window menu. The help window will appear, displaying information related to the input card currently open. Click on the Find button, type "van Genuchten" in the Find Info... field, and then press the [RETURN] key. The help window will display the van Genuchten equations (Figure 5.10). Information about many other topics may be found through online help. When finished, click the Ok button to close the help window. Accept your input entry and navigate to the next card (Liquid Relative Permeability).

5.4.8 Liquid Relative Permeability

Choose Generic Sand from the Rock List. Select the Mualem w/ van Genuchten option to compute relative permeability, and enter the value of the parameter m. If you do not know how to compute the value of m, check the help window on van Genuchten again where the value of m is defined (remember, $n = 1.5$ for this problem; use the equation you see in the help screen to compute m and enter that value). Finally, enter a minimum liquid relative permeability of 1.0×10^{-10} m (1.0E-10). Accept your entry and navigate to the Liquid Boundary Conditions card.

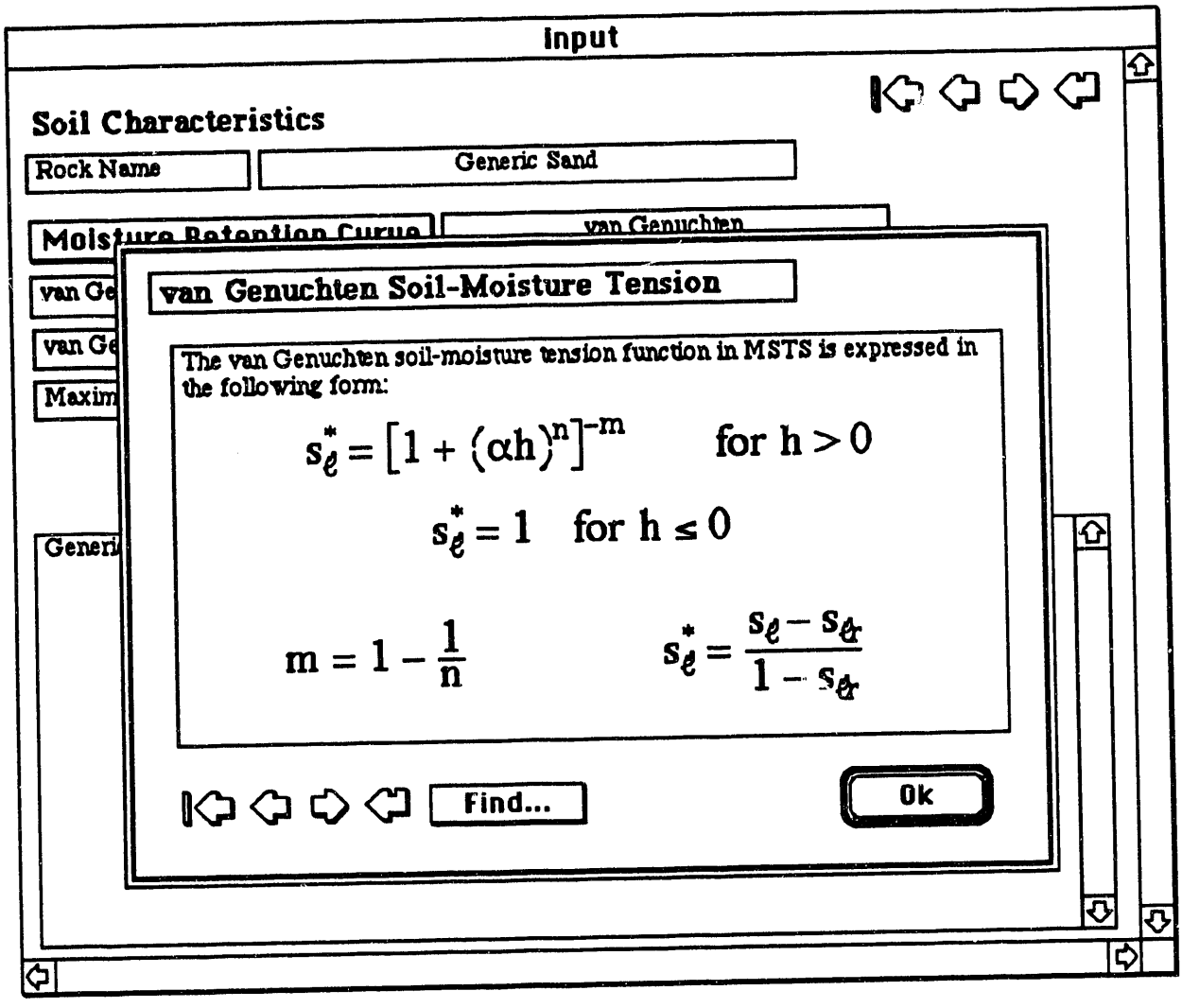

Figure 5.10. Example of MSTS Graphical Input Interactive Help Feature

5.4.9 Liquid Boundary Conditions

The quick tour problem involves a fixed water recharge of 1.0 cm/h at the top of the column and saturated conditions at the column bottom. To specify the top boundary condition as constant recharge, choose Z-Direction: Top Surface from the Orientation Index button menu and click the Entire Surface button. Choose the Neumann @ Boundary condition from the Boundary Type button menu. The mass flux is computed by multiplying the volumetric recharge of 1.0 cm/h by the density of water (998.32 kg/m^3 at 20°C), as follows:

$$\text{Mass Flux Rate} = \left(1.0\ \frac{\text{cm}}{\text{h}}\right)\left(\frac{1\ \text{m}}{100\ \text{cm}}\right)\left(\frac{1\ \text{h}}{3600\ \text{s}}\right)\left(998.32\ \frac{\text{kg}}{\text{m}^3}\right) = 2.773 \times 10^{-3}\ \text{kg/m}^2\text{s}$$

Type 2.773E-3 in the Field Variable field to represent the liquid mass flux and enter 998.32 kg/m^3 as the liquid density (remember to select the appropriate units!). The air mass fraction may be neglected for this problem. Accept the entry. For the lower boundary, choose the appropriate index (Z-Direction: Bottom), click the Entire Surface button, and select "Saturated @ Boundary" as the boundary type. Enter the same liquid density as before and accept this entry also. Check that there are two lines in the scrolling box at the bottom of the input card that look like this:

```
Z-Direction: Top Surface,Neumann @ Boundary,2.773E-3,kg/m^2 s,998.32,kg/m^3,,1,1,1,1,20,20
Z-Direction: Bottom Surface,Saturated @ Boundary,,,998.32,kg/m^3,,1,1,1,1,1,1
```

The liquid boundary conditions are now prescribed. Because the quick tour problem does not require boundary conditions for vapor, gas, energy, or species transport and there are no sources or sinks specified for this problem, we will skip the other boundary condition cards and the Sources and Sinks card. Navigate to the Initial Conditions card.

5.4.10 Initial Conditions

The initial state for hydrologic conditions can be completely defined by specifying any pair of the following field variables: gas pressure, liquid pressure, and liquid saturation. The unspecified field variable will by computed by MSTS from the water-retention characteristic function. Choose the option "Liquid Saturation & Gas Pressure" from the button menu labeled "Initial Saturation Option" to indicate how initial conditions will be specified for this problem. Specify the first field variable by choosing "Gas Pressure" from the button menu labeled "Field Variable" and click the Entire Domain button to specify the nodes to be initialized. The initial gas pressure throughout the domain will be atmospheric, so enter 101325.0 into the Gas Pressure box and select "Pa (abs)" from the Unit button menu. Leave the gradients at zero (uniform initial conditions). Accept this entry and observe the new line added to the scrolling box below:

```
Gas Pressure,101325.0,Pa (abs),0.0,1/m,0.0,1/m,0.0,1/m,1,1,1,1,1,20,
```

The liquid saturation is specified in the same way; change the field variable to "Liquid Saturation" using the Field Variable button menu and enter 0.50 for the liquid saturation. The entire domain is still set from the liquid pressure entry, so accept this entry and a second line is recorded:

```
Liquid Saturation,0.50,,0.0,1/m,0.0,1/m,0.0,1/m,1,1,1,1,1,20,
```

These two lines together set the initial hydrologic conditions for our problem. We have not specified an initial temperature, so MSTS will initialize the domain to 20°C. Navigate to the Output Control card.

5.4.11 Output Control

The Output Control card provides flexibility in the type and quantity of output produced by MSTS during a simulation. Three scrolling field boxes appear on the left side of the Output Control card (Figure 5.11) that display the field variables to be recorded to the three output devices: the output file, the plot file, and the reference node output. The reference node is limited to a maximum of seven field variable outputs. The output and plot files may contain any number of field variables. To modify the field variables in each scrolling box, click on the radio button corresponding to the output device and a listing of possible field variables will appear. Click the check box next to each desired field variable to select that variable for output (click again to deselect any you do not want) and click the Ok button when finished. Practice now by choosing liquid pressure, liquid saturation, total hydraulic head, volumetric moisture content, and z-direction liquid velocity for all three output devices (output, plot, and reference node). We will want output for the whole problem, so click the Entire Domain button and click the Z-X Planes radio button to indicate the orientation for output. It is possible to request output at several simulation times, but we will settle for the final condition at the end of the simulation: enter 2.0 and select "h" as the time unit for field variable output times. Accept this entry. Up to four reference nodes can be monitored during a simulation execution. We will use one for this tour; enter 1 for x, 1 for y, and 20 (the top) for z. This causes the values to be displayed at every time step for all of the field variables chosen above for node (1,1,20).

5.5 Saving an Input File

To save the completed input file, press ⌘S (or select Save from the File menu). Make sure that you use the name "input" for the saved file. While the file is being written, a "Writing Input File" message will be displayed indicating the recording progress. Although you were not directed to do so in this tour, it is wise to save the input file frequently while you develop it with the Graphical Input to prevent loss in case of a power failure, a machine freeze, or other interruption that could lose all entries to that point.

5.6 Parameterization and Machine Specification

Although you have an input file now, you must still determine how large the parameters must be in the MSTS code. The Graphical Input provides a quick way to do this: select "Compute Parameters" from the Resource menu. The Graphical Input will prompt you to choose an input file:

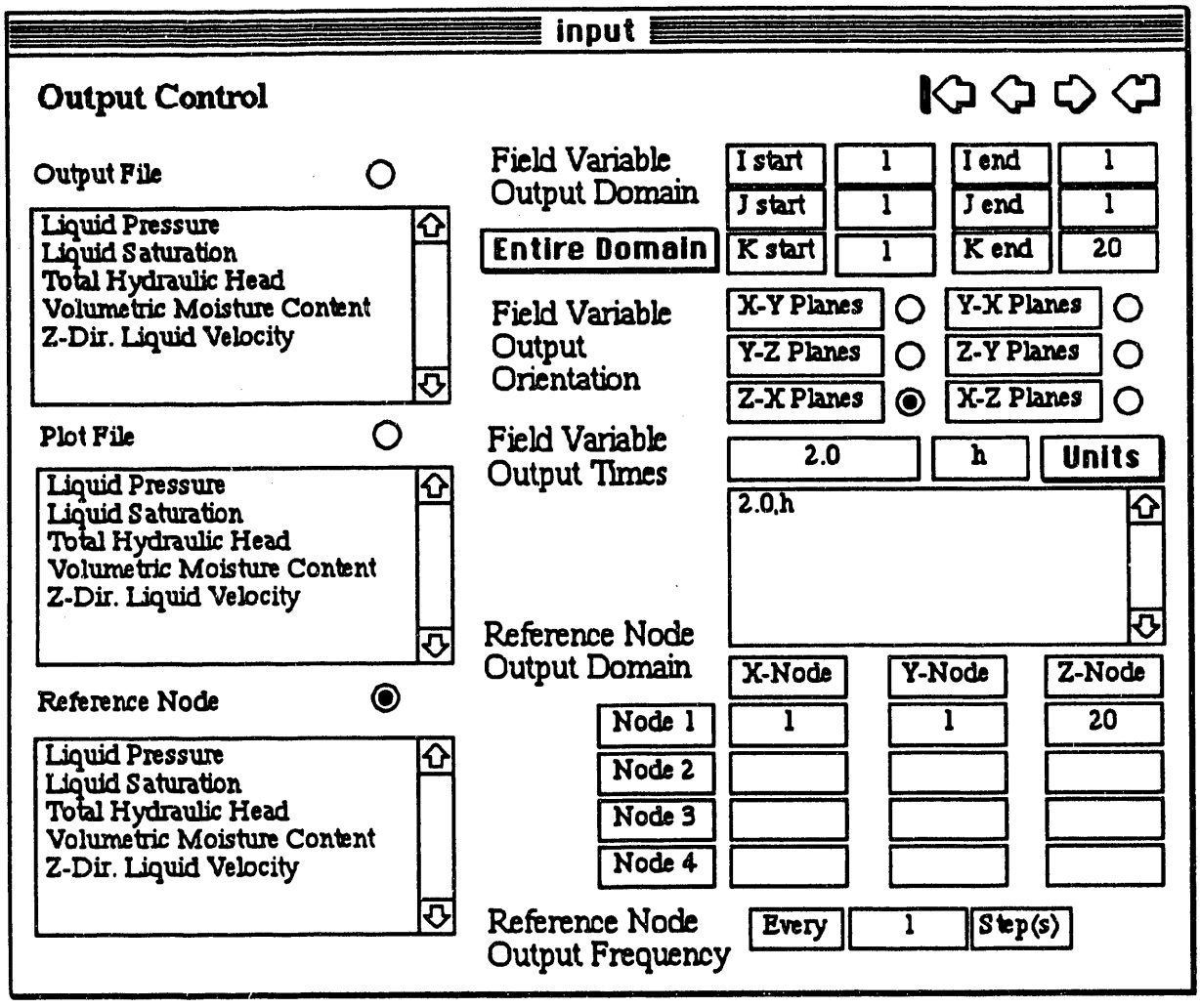

Figure 5.11. Output Control Input Card from MSTS Graphical Input

pick the file "input" that you just saved. The Graphical Input will proceed to read the input file and compute the minimum size for each MSTS parameter (refer to Section 4.0 for details on parameters) for this input file. The results will be displayed on the screen (Figure 5.12) and recorded in the default directory in the file "parameter". You are now finished using the Graphical Input; close it by clicking the Ok button on the parameter display, then choosing Quit from the File menu. Choose No when prompted if you wish to save the input file (you have made no changes since saving it last). With this, your Graphical Input session is closed.

Next you must parameterize the MSTS code. Using your preferred text editor, open the file "msts.f" and locate the first block of parameter statements (within the first 100 lines of code). This parameter block is repeated throughout the code in exactly the same way, so we can use the search-

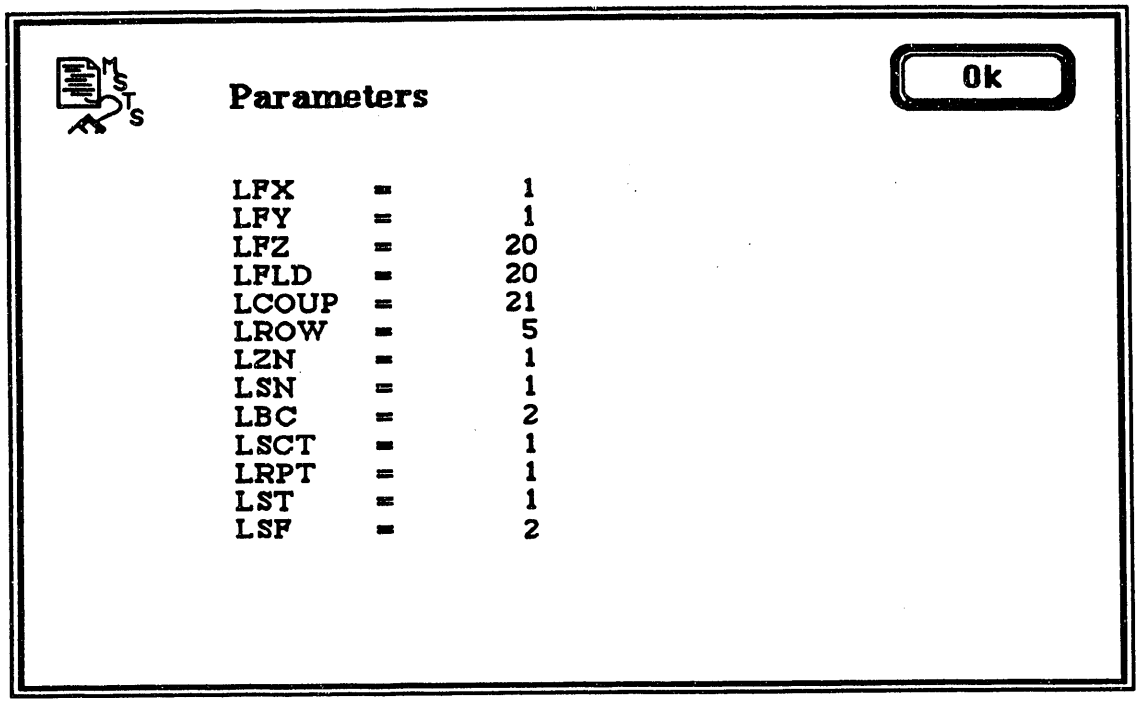

Figure 5.12. Example of the "Compute Parameters" Resource of the MSTS Graphical Input

and-replace feature of your text editor to make parameterization easy. Search for all occurrences of the first three (not all five) parameter statements, and replace them with the three parameter statements you will find in the file "parameter" that was written by the Graphical Input.

To make the code machine-specific, search for a set of comment lines that pertain to your code and delete them. Assuming you will run the MSTS code for this tour on your Macintosh computer, search for all occurrences of "CMAC" and delete these. This will make active statements out of the time and date functions MSTS requires that vary from one computing environment to another. Other machines have different comment lines to alter: "CRAY" for the Cray computer, "CSUN" for a Sun workstation, and so on (see Section 4.0 for a complete listing of these). When finished deleting the "CMAC" occurrences, save the "msts.f" file. (Important: be careful you save an original, unaltered copy of the "msts.f" file!) The code is now parameterized and specific to your computer. It is important to save the original "msts.f" file because making it machine-specific by altering a fresh copy of the original each time is easier than trying to restore one set of comments and deleting another (e.g., restoring all the "CMAC" occurrences and deleting all the "CSUN" occurrences to prepare for a simulation on a Sun workstation is more difficult than merely deleting the "CSUN" occurrences on a new copy).

5.7 Running a Simulation

Ensure that the "input" and "msts.f" files you have prepared are in the default directory you wish to use for the simulation. Compile the "msts.f" using the FORTRAN compiler you have available. Then invoke the application (executable file); no other action is required. MSTS will read the file "input" and follow its instructions.

5.8 Examining Output

General simulation output is contained in the "output" file, which is in ASCII format and may be viewed with the text editor of your choice. The output file contains a unique run-identification number and the time and date of the run as well as an "echo" of the information read from the input file. Check the first part of the output file to ensure that the input information repeated there is what you entered using the Graphical Input. Next, the output file records the reference node information just as it appeared on the screen during the simulation execution. Finally, the field variables you requested in the Output Control card of the input file are recorded.

Most often you will wish to graph the results of your simulation or prepare images (contour plots or raster images) of the results. The "plot" file generated by MSTS makes this easier to do. Any field variables separately requested for the plot file are recorded in a format more conducive to plotting tasks. Following some header information, the names of the variables in the plot file are listed (one per line), followed by a listing of the field variables in increasing node order. The node number and x-, y-, and z-coordinates of the node are always provided in the first four columns and the node volume in the fifth column.

5.9 More Sample Problems

Additional sample problems can be found in Section 8.0. The samples include single-node evaporation and condensation tests, a heat pipe problem, flow from hot two-phase conditions, vertical and horizontal infiltration problems, and an unsaturated transport problem.

6.0 Input File Structure

Control and model parameter specification is accomplished in MSTS through the "input" file. An "input" file may be prepared either by using the MSTS Graphical Input (see Section 3.0 for details) or by using a text editor and complying with the MSTS input file format requirements. This section provides detailed information for each card in an MSTS input file and is intended as a reference. The typical MSTS user will commonly use the Graphical Input and therefore not need to be intimately familiar with all the details provided in this section but may refer to them as needed.

This section is grouped by card function (e.g., all of the cards that are used to specify boundary conditions are together), and the cards are organized in the same order as in an MSTS input file. Table 6.1 summarizes all of the input cards contained in an MSTS input file in this order.

The "input" file itself must be an ASCII file and hence is portable between computing environments. Therefore, a user may prepare an "input" file on a personal computer, transfer the file to a mainframe, and run the simulation. The syntax rules used in this section are presented in Table 6.2. MSTS avoids case-sensitive errors by converting all input file contents to lower case as the input is received by the code. Very little other error checking is performed on the input; hence close attention to the format requirements presented in this section is necessary. The easiest way to avoid format errors is to use the MSTS Graphical Input to prepare input files, as that application is specifically designed to comply with all of the format requirements contained in this section.

Table 6.1. MSTS Input Cards

Input Card	Information Specified
Simulation Title	identification of simulation, user, notes, file creation time and date
Solution Schemes	solution scheme, governing equations, simulation time control
Numerical Control	iteration limits, convergence criteria, averaging techniques
Grid Geometry	coordinate system, physical extent, number and location of nodes
Inactive Nodes	location of noncomputational nodes
Rock or Soil Types	identification of rock or soil types and node assignment
Mechanical Properties	porosities and tortuosities
Hydraulic Properties	hydraulic conductivities (or permeabilities)
Thermal Properties	thermal conductivities, rock or soil density, heat capacity
Species Properties	identification of species, decay rates, coefficients
Soil Characteristics	moisture-retention characteristics, tension head limits
Liquid Relative Permeability	unsaturated liquid relative-permeability parameters
Gas Relative Permeability	gas relative-permeability parameters
Liquid Boundary Conditions	type, extent, and magnitude of boundary conditions for liquid water
Gas Boundary Conditions	type, extent, and magnitude of boundary conditions for gas
Vapor Boundary Conditions	type, extent, and magnitude of boundary conditions for vapor
Energy Boundary Conditions	type, extent, and magnitude of boundary conditions for thermal energy
Species Boundary Conditions	type, extent, and magnitude of boundary conditions for species mass
Initial Conditions	specification of field variable initial values
Sources and Sinks	location, temporal variation, and strength of sources and sinks
Liquid Pathline Trace	liquid pathlines for which pathline and travel times are required
Output Control	field variables to record in output files
Surface Flux Integrator	planes to report fluxes of mass or energy as a function of time

Table 6.2. Input Reference Conventions

Notation	Interpretation
Line 1	The first line in an input card following the card name.
Line n	One of N line(s) in an input card, where N is declared in the beginning of the input card and $1 \leq n \leq N$.
~	A tilde always precedes the name of an input card and signals the input modules of MSTS to the beginning of a new input card.
,	Commas separate individual entries in a line within an input card. A terminating comma is usually required at the end of each line (inclusion of a terminating comma where it is not required does not adversely affect input).
I, J, K	Indices for node ranges in the *x*-, *y*-, and *z*-directions for Cartesian coordinate systems, or indices for node ranges in the *r*-, θ–, and *z*-directions for cylindrical coordinate systems.
[x | y]	Square brackets indicate a list of options separated by vertical lines. Only one of the available options may be used and must be written precisely as shown in the option list except that the case of characters is unimportant (Aa, aa, and AA are all equivalent).
{ alpha }	Braces enclosing the word "alpha" indicate field inputs of alphabetic characters.
{ alpha-numeric }	Braces enclosing the words "alpha-numeric" indicate field inputs of alphabetic and numeric characters.
{ integer }	Braces enclosing the word "integer" indicate field inputs of integer numbers.
{ real }	Braces enclosing the word "real" indicate field inputs of real numbers.
(text)	Text within parentheses gives informal directions on what type of line, or group of lines, may be used in an input card.
text	Italicized text defines input options.
"text"	Text within the quotation marks is to be typed <u>exactly</u> as shown, except that the case of characters is unimportant (Aa, aa, and AA are all equivalent).

Table 6.2. (Contd)

Notation	Interpretation
`text`	Courier typeface is used to display text from any computer file, such as an input file. In some cases, a line in a computer file is wider than can be displayed within the margins of this document, in which case the additional text is shown on subsequent indented line(s) to signify that it is a continuation of the same line. To illustrate:

```
~Example Input Card
1 line of example input follows.
This is a single line in the input file but is too wide for the
      margins of this reference, so the continuation of the line is
      indented to indicate that it is actually one line.
```

6.1 Simulation Documentation and Control

Simulation documentation and control are accomplished with the Simulation Title, Solution Schemes, and Numerical Control cards. The first card provides a way to identify each "input" file by title, user, date and time of creation, and MSTS version name and revision number. The Solution Schemes card is used to specify which combination of the four governing equations (thermal energy conservation, water conservation, air conservation, and species mass conservation) is to be solved, the period of time to be simulated, and the solution scheme (e.g., banded matrix). The Solution Schemes card also provides control over other options like debugging output, screen echoing during a simulation, binary diffusion, etc. The Numerical Control card is used to enter convergence criteria, averaging options, computer time limits, and iteration limits.

6.1.1 Simulation Title Card

Function

The Simulation Title card is used to specify information that uniquely identifies an "input" file, including the title of the simulation, the user's name and affiliation, the "input" file creation date and time, and any notes the user may enter.

Format

Line 0	"~Simulation Title and Notes"
Line 1	Version Name { alpha (4 characters) }, Revision Number, { integer (4 digits) }
Line 2	Simulation Title { alpha-numeric },
Line 3	User Name { alpha-numeric },
Line 4	Company Name { alpha-numeric },
Line 5	"Input" File Creation Date { alpha-numeric (20 characters maximum) },
Line 6	"Input" File Creation Time { alpha-numeric (20 characters maximum) },
Line 7	Characters { integer } "character(s) of simulation title notes follows."
Line(s) 8+	Simulation Title Notes { alpha-numeric (80 characters per line, no returns) }

Comments

The version name and release number provide positive identification of the particular MSTS code used, preventing use of inconsistent MSTS Graphical Input and MSTS code versions. The version name (e.g., "beta") and release number (e.g., "0001") pertain to both the MSTS code itself and the MSTS Graphical Input. The MSTS Graphical Input will accept only files that have the same version name and release number.

The Simulation Title field is a short, one-line description or title that will allow the user to quickly recognize which simulation is controlled by this "input" file. The User Name and Company Name fields are provided for additional background information. The Simulation Title Notes field provides a space to enter a more extensive description of the "input" file.

Examples

In this example a vertical infiltration problem is identified. The input card belongs to a file created with the beta version of MSTS, release 0001. The file creation date and time are indicated,

and a short description of the problem is included in the Simulation Title Notes field.

```
~Simulation Title and Notes
beta,0001,
Philip's Vertical Infiltration Problem
W. E. Nichols
Battelle, Pacific Northwest Laboratory
Thursday, June 4, 1992
1:08:41 PM
200 character(s) of simulation title notes follows.
The objective of this test problem is to verify that the water conservation equa
tion of MSTS correctly computes the wetting front of the one-dimensional, time-d
ependent, unsaturated pressure equation.
```

6.1.2 Solution Schemes Card

Function

The Solution Schemes card is used to invoke restart options, control simulation time variables, select a matrix solution scheme, specify which governing equations to solve, choose secondary process options, and invoke debugging assistance options.

Format

Line 0	"~Solution Schemes"
Line 1	Initial Conditions Only [true | false], Restart [true | false], Restart from Time Zero [true | false],
Line 2	Matrix Solution Scheme [banded matrix | conjugate gradient],
Line 3	Energy Equation [true | false], Water Equation[true | false], Air Equation [true | false], Species Concentration Equation [true | false],
Line 4	Simulation Time Limit { real }, Units [s | min | h | day | wk | yr],
Line 5	Initial Time Step { real }, Units [s | min | h | day | wk | yr],
Line 6	Time Step Acceleration Factor { real },
Line 7	Maximum Time Step { real }, Units [s | min | h | day | wk | yr],
Line 8	Screen Echo [true | false], Binary Diffusion [true | false], Fixed Properties [true | false], Liquid Phase [true | false], Gas Phase [true | false], Vapor Pressure Lowering [true | false],
Line 9	Print Subroutine Names [true | false], Print Matrix Arrays [true | false], Print Timing Information [true | false], Undefined [true | false],

Comments

The Initial Conditions Only option, when invoked (true), will force MSTS to read the "input" file, compute all secondary variables and fluxes (e.g., liquid saturation and Darcy velocities), and stop execution. This option is useful if the user wishes to confirm that the initial conditions are correct before proceeding with a lengthy simulation.

The Restart option permits a restart from a previous simulation. Whenever a simulation is completed, MSTS records a file named "restart," which can be read to begin a new simulation from the same conditions. To invoke this option, set the Restart option to "true" and ensure that a valid "restart" file is available in the same directory as the "input" file. The Restart from Time Zero option applies only to restarted simulations. If the Restart from Time Zero option is set to "true," then the simulation time begins at zero for a simulation where the initial conditions are taken from the "restart" file; if set to "false," then the time continues from the simulation time of the "restart" file.

The governing equations for conservation of component mass and thermal energy are considered coupled equations. Seven solution modes or combinations of the coupled conservation equations are available with MSTS. Refer to Section 2.4 for a description of the seven solution modes. Solution of the species conservation equation can be appended to any of the seven coupled-equation solution modes.

Examples

In this example, a simulation is started from initial conditions specified in the "input" file (not a "restart") and is solved using the banded matrix solution scheme. Only the water conservation equation will be solved for a simulated time of 2 hours beginning with an initial time step of 0.01 hour with a time-step acceleration factor of 1.25 (i.e., each time step will be 1.25 times larger than the previous unless the convergence criterion is violated), up to a maximum time step of 0.10 hour. A screen echo of the progress of the simulation will be available, binary diffusion is not included, and fluid properties are fixed (usually this is chosen for isothermal problems only). The liquid phase will be simulated, but not the gas phase. The vapor-pressure-lowering feature is not activated either. No debugging output is requested (subroutine names, array output, or timing information).

```
~Solution Schemes
false,false,false,
banded matrix
false,true,false,false,
2,h,
0.01,h,
1.25,
0.10,h,
true,false,true,true,false,false,
false,false,false,false,
```

We can modify the same example for a second simulation in which thermal effects and the gas phase are modeled. In this case, we invoke two more equations (line 3), switch the Fixed Properties option to "false" because fluid properties will change with temperature, and switch the Binary Diffusion, Gas Phase, and Vapor Pressure Lowering options to "true," as follows:

```
~Solution Schemes
false,false,false,
banded matrix
true,true,true,false,
2,h,
0.01,h,
1.25,
0.10,h,
true,true,false,true,true,true,
false,false,false,false,
```

6.1.3 Numerical Control Card

Function

The Numerical Control card is used to control the iteration process, constrain the use of computer resources (limits on both total CPU usage and actual time), and specify the numerical convergence limits and averaging technique used for solution of each of the governing equations.

Format

Line 0	"~Numerical Control"
Line 1	Number of Newton-Raphson Iterations { integer }, Residuals Convergence [least squares | maximum residual],
Line 2	CPU Execution Time Limit { real }, Units [s | min | h | day | wk | yr], Clock Time Limit { real }, Units [s | min | h | day | wk | yr],
Line 3	Thermal Energy Equation Convergence Criterion { real }, Water Equation Convergence Criterion { real }, Air Equation Convergence Criterion { real },
Line 4	Thermal Energy Equation Mean [harmonic | geometric | arithmetic | upwind], Water Equation Mean [harmonic | geometric | arithmetic | upwind], Air Equation Mean [harmonic | geometric | arithmetic | upwind], Species Concentration Equation Mean [harmonic | geometric | arithmetic | upwind],

Comments

The CPU execution time and clock time limits are provided to give a user the means to prevent a batch-process run of the MSTS code from exceeding queue limits in a mainframe computer. For example, if the host computer queue limits a batch submission to 4 CPU-hours, the CPU execution time limit can be set to 3.9 hours to prevent an interruption. MSTS will execute for 3.9 hours and write the requested output files for the last time step completed at that time, including a "restart" file. If additional time is required to finish the simulation, the "restart" file can then be used to continue. The clock time limit works in the same manner.

Convergence limits need be specified only for those coupled governing equations that are to be solved, as indicated by options in the Solution Schemes card.

Examples

For this example, we choose to specify eight Newton-Raphson iterations using the Maximum Residual Convergence option. The simulation will be stopped and a "restart" file written for possible later use if the simulation consumes more than 1 hour of CPU time or 5 hours of wallclock time. The Convergence Criterion field for each of the three coupled governing equations is 1.0×10^{-6}, and all internodal properties will be computed using a harmonic mean.

```
~Numerical Control
8,Maximum Residual,
1,h,5,h,
1.0E-06,1.0E-06,1.0E-06,
Harmonic Mean,Harmonic Mean,Harmonic Mean,Harmonic Mean,
```

The first example could be modified to allow 10 Newton-Raphson iterations per time step, extend the CPU execution limit to 6 hours, extend the clock limit to 1 day, and require a geometric mean for solution of the water conservation equation, as follows:

```
~Numerical Control
10,Maximum Residual,
6,h,1,day,
1.0E-06,1.0E-06,1.0E-06,
Harmonic Mean,Geometric Mean,Harmonic Mean,Harmonic Mean,
```

6.2 Computational Domain

The computational domain is defined using the Grid Geometry, Inactive Nodes, and Rock or Soil Types cards. The first of these, Grid Geometry card, is used to specify the coordinate system (Cartesian and cylindrical are available), the total physical length of the model domain in each dimension, the number of nodes in each dimension, the elevation datum, and the location of each node. Often the rectangular grid required by the finite-difference method used in MSTS does not provide the flexibility needed to describe complex geometries; the Inactive Nodes card provides a way to "blank out" noncomputational nodes, which MSTS will not treat as a part of the porous media continuum in a simulation. The inactive nodes feature is useful, for example, when modeling a geometry in which several nodes in the corner of a model domain are in the atmosphere; impervious regions also could be modeled as inactive nodes. The Rock or Soil Types card is used to assign ranges of nodes to a rock or soil type. The rock or soil type is commonly identified by a name, such as "Ringold Formation" or "Willamette Silt Loam." All physical properties of these rock or soil types are defined in subsequent input cards and assigned to the type by the identifying name.

6.2.1 Grid Geometry Card

Function

The Grid Geometry card is used to select the problem coordinate system (Cartesian or cylindrical), specify the number of nodes, specify the physical extent of the problem domain, and indicate the physical location of all nodes in the problem domain.

Format

Line 0	"~Grid Geometry"
Line 1	Coordinate System [Cartesian | cylindrical],
Line 2	Number of Grid Nodes in the x- or r-Direction { integer }, Number of Grid Nodes in the y- or θ-Direction { integer }, Number of Grid Nodes in the z-Direction {integer },
Line 3	x- or r-Direction Physical Domain Length { real }, Units [m | ft | cm], y- or θ-Direction Physical Domain Length or Arc { real }, Units [m | ft | cm | degrees], z-Direction Physical Domain Length { real }, Units [m | ft | cm], z-Direction Datum z^* { real }, Units [m | ft | cm], z-Direction Grid Bottom Elevation from Datum { real }, Units [m | ft | cm],
Line 4	Inner Radius Length r_0 { real (cylindrical coordinates; enter zero for Cartesian) }, Units [m | ft | cm],
Line 5	I { integer } "line(s) of grid geometry input follows."
Line i	"Node " i { integer }, x- or r-Direction Node Position { real }, Units [m | ft | cm],
Next Line	J { integer } "line(s) of grid geometry input follows."
Line j	"Node " j { integer }, y- or θ-Direction Node Position { real }, Units [m | ft | cm | degrees],
Next Line	K { integer } " line(s) of grid geometry input follows."
Line k	"Node " k { integer }, z-Direction Node Position { real }, Units [m | ft | cm],

Comments

The Cartesian coordinate system is used to represent any length, area, or volume in rectangular grid volumes. Cartesian coordinates always imply the horizontal plane is represented by x- and y-axes, and the vertical plane (coinciding with the gravity vector) by the z-axis. The cylindrical coordinate system can be used to represent a radial, symmetric problem only, centered on a point. The horizontal plane in this case is represented by the radius r and angle θ. The vertical plane is represented by the z-axis, just as for Cartesian coordinates. Any portion of an arc greater than 0 degrees but less than 360 degrees may be represented with cylindrical coordinates, though the symmetry requirement would imply that a smaller, representative arc would be sufficient for most radial problems.

Node positions are referenced from the west, south, or bottom boundaries for the x-, y-, and z-coordinate directions, respectively, for Cartesian coordinate systems. For cylindrical coordinate systems, node positions are referenced from the west, south, or bottom boundaries for the r-, θ-, z-coordinate directions, respectively. Surfaces between nodes are located at the midpoint between two adjacent node positions. Node volumes are defined by their bounding surfaces. To illustrate, a one-dimensional problem 3 m in length could be represented by three uniformly distributed nodes in the appropriate dimension, located at 0.5, 1.5, and 2.5 m, as shown in Figure 6.1. For a nonuniform distribution of nodes, a node is not necessarily centered in the grid cell it represents. Figure 6.2 illustrates the same one-dimensional, three-cell problem of 3-m length represented by nonuniform node spacing at 1.0, 1.5, and 2.5 m. The first grid cell, which is the length represented by node 1, extends from the left domain boundary ($x = 0$) to the midpoint between the first and second nodes ($x = 1.25$ m).

In MSTS, the physical position of every node must be a positive number. MSTS grid geometries should generally arrange a grid such that the lower boundary in each dimension is at position zero. The vertical dimension can be offset to a different reference by means of the z-Direction Grid Bottom Elevation from Datum field value. For example, if the bottom of a model domain is at elevation 700 m above mean sea level and the top is at 1000 m, distribute z-direction nodes from zero to 300 m in the K dimension and assign a value of 700 m to the z-Direction Grid Bottom Elevation from Datum field.

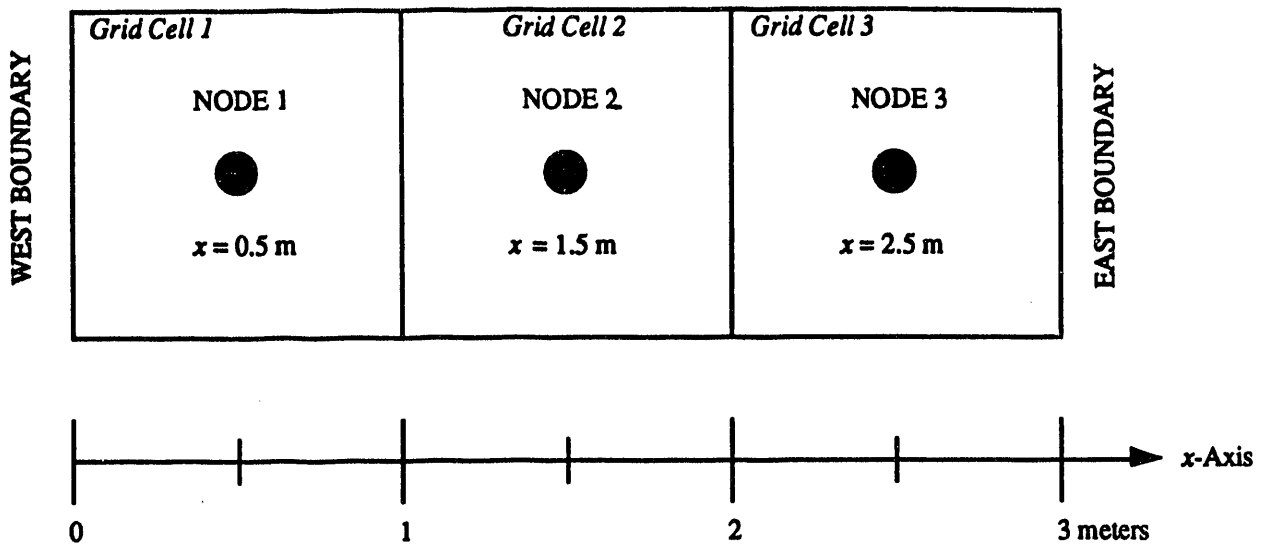

Figure 6.1. Example Grid Nodes and Associated Grid Cells for Uniform Node Distribution

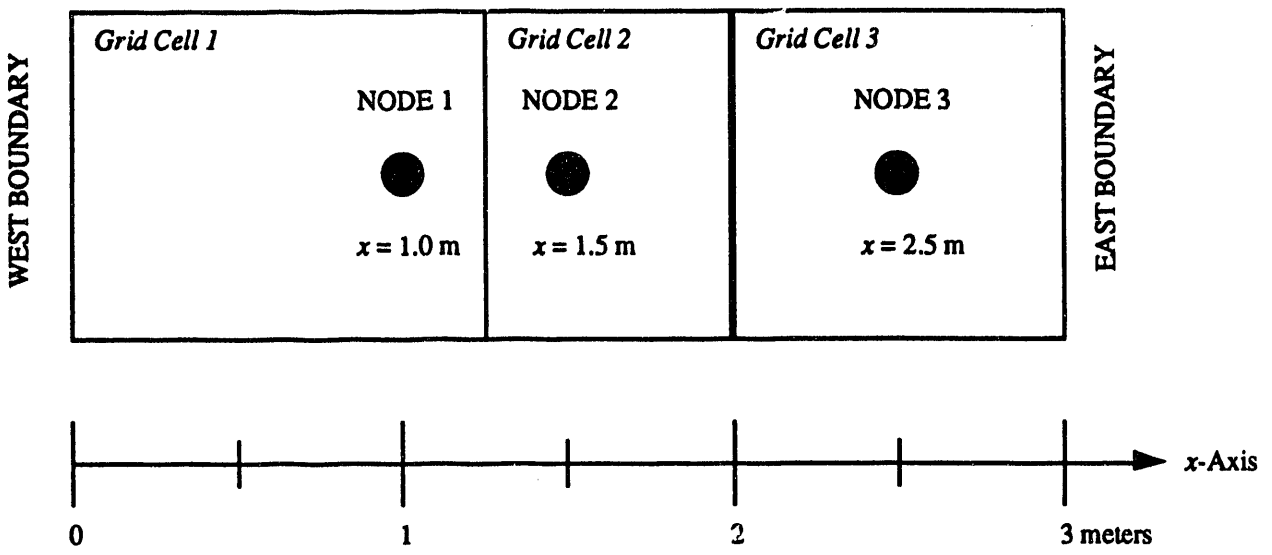

Figure 6.2. Example Grid Nodes and Associated Grid Cells for Nonuniform Node Distribution

Examples

The first example shows how the problem illustrated in Figure 6.1 would be defined using the Grid Geometry card. This problem is a single-dimension (in the x-direction) domain 3 m in length to be represented by three nodes. The y- and z-direction nodes are given a single node each to indicate the one-dimensional aspect of the problem.

```
~Grid Geometry
```

```
cartesian
3,1,1,
3.0,m,1.0,m,1.0,m,0.0,m,0.0,m,
0.0,m,
3 line(s) of grid geometry input follows.
Node 1,0.5,m,
Node 2,1.5,m,
Node 3,2.5,m,
1 line(s) of grid geometry input follows.
Node 1,0.0,m,
1 line(s) of grid geometry input follows.
Node 1,0.0,m,
```

A vertical domain is similar, except the *z*-axis is the multiple node direction. The next example illustrates use of the Grid Geometry card for a one-dimensional (vertical), five-node problem that models a physical length of 10.0 cm. The top of the domain is taken as elevation zero, so the bottom of the domain is at elevation -10.0 cm.

```
~Grid Geometry
cartesian
1,1,5,
1,cm,1,cm,10.0,cm,0.0,cm,-10.0,cm,
0.0,m,
1 line(s) of grid geometry input follows.
Node 1,0.5,cm,
1 line(s) of grid geometry input follows.
Node 1,0.5,cm,
5 line(s) of grid geometry input follows.
Node 1,1.0,cm,
Node 2,3.0,cm,
Node 3,5.0,cm,
Node 4,7.0,cm,
Node 5,9.0,cm,
```

For a radially symmetric, 10-m-tall, 1-m-radius problem centered on a borehole with inner radius 10 cm and represented by a 10-degree arc, the Grid Geometry card would look like:

```
~Grid Geometry
cylindrical
5,1,5,
1,m,10,degrees,10,m,0.0,m,0.0,m,
10.0,cm,
5 line(s) of grid geometry input follows.
Node 1,0.1,m,
Node 2,0.3,m,
Node 3,0.5,m,
Node 4,0.7,m,
Node 5,0.9,m,
1 line(s) of grid geometry input follows.
Node 1,5,degrees,
5 line(s) of grid geometry input follows.
Node 1,1,m,
Node 2,3,m,
Node 3,5,m,
Node 4,7,m,
Node 5,9,m,
```

6.2.2 Inactive Nodes Card

Function

The Inactive Nodes card is used to designate inactive, or noncomputational, nodes in the problem domain. Inactive nodes may represent any portions of the model domain that are to be excluded from the porous media continuum to be simulated. Examples might include nodes representing the atmosphere or impervious rock. Inactive nodes can also be used to define internal boundary conditions. A surface between an inactive and an active node can function as a boundary surface for the active node. Normal boundary conditions may be applied to these internal surfaces.

Format

Line 0	"~Inactive Nodes"
Line 1	N { integer } " line(s) of inactive nodes input follows."
Line n	I Start { integer }, I End { integer }, J Start { integer }, J End { integer }, K Start { integer }, K End { integer },

Comments

The restriction to rectangular elements imposed by the finite-difference method used in the MSTS code makes descriptions of irregular geometries difficult. The inactive nodes feature of MSTS gives some flexibility in this regard by allowing the user to specify nodes at which the governing equations will not be solved and which can be assigned boundary conditions. Although grid cells are still restricted to rectangular elements, the model domain is not. Examples of appropriate uses for inactive nodes include representation of the atmosphere for a sloping surface at the upper part of a model, representation of a nonhorizontal saturated zone in a unsaturated model domain, and representation of impervious zones within a model domain.

Examples

This example makes two groups of nodes inactive; one group will represent the atmosphere in the upper left-hand portion of a two-dimensional (10 by 1 by 5 node) domain, and the other group will represent an impervious region in the lower left-hand portion.

```
~Inactive Nodes
2 line(s) of inactive nodes input follows.
8,10,1,1,5,5,
1,3,1,1,1,2,
```

The following example declares that there are no inactive nodes in the model domain:

```
~Inactive Nodes
0 line(s) of inactive nodes input follows.
```

6.2.3 Rock or Soil Types Card

Function

The Rock or Soil Types card is used to group computational node(s) with identical physical properties into unique rock or soil types.

Format

Line 0	"~Rock or Soil Types"
Line 1	Characters { integer } "character(s) of rock or soil types notes follows."
Line 2+	Rock Notes { alpha-numeric (strictly 80 characters per line) }
Next Line	M { integer } " line(s) of rock or soil types input follows."
Line m	Rock or Soil Type { alpha (80 characters maximum) }, I Start { integer }, I End { integer }, J Start { integer }, J End { integer }, K Start { integer }, K End { integer },

Comments

The Rock Notes field is used to include references or sources of information that help in documenting where the user obtained the properties used to represent rock or soil types.

The Rock or Soil Types card is used to specify properties for similar groups of nodes, often termed zones, units, or layers. Usually groupings follow hydrogeologically similar soils or rock formations. The Rock or Soil Type field is a name that identifies the grouping to which properties are assigned, e.g., "Tiva Canyon Welded" or "Yolo Light Clay." The next six numbers bound the rectangular block of nodes that are assigned to that rock or soil type. Multiple lines can be used to assign different groups of nodes to the same rock type (see the following examples).

Examples

In the first example, a one-dimensional vertical column of Yolo light clay is specified as the only soil type in the simulation and all 100 nodes of the problem are assigned to this type:

```
~Rock or Soil Types
52 character(s) of rock or soil types notes follows.
Yolo light clay was first described by Moore (1939).
1 line(s) of rock or soil types input follows.
Yolo Light Clay,1,1,1,1,1,100,
```

Often it is necessary to use multiple lines to assign all of the nodes belonging to one rock or soil type. Here the first example is repeated with a middle layer of 21 nodes assigned to a different rock type (generic sand):

```
~Rock or Soil Types
52 character(s) of rock or soil types notes follows.
Yolo light clay was first described by Moore (1939).
3 line(s) of rock or soil types input follows.
Yolo Light Clay,1,1,1,1,1,39,
Generic Sand,1,1,1,1,40,60,
Yolo Light Clay,1,1,1,1,61,100,
```

6.3 Physical Properties

Physical properties include mechanical properties (porosity and tortuosity), hydraulic properties (permeability or conductivity, and storativity), thermal properties (thermal conductivity, density, and specific heat), species properties (species name, molecular diffusion, liquid-gas partition coefficient, solid-liquid partition coefficient, and species half-life), soil characteristics (moisture-retention relations), liquid relative permeability, and gas relative permeability. All of the physical characteristics of a rock or soil type used by the MSTS code are entered using these seven physical properties input cards. In each card, the physical properties are assigned to a rock or soil name that must match precisely (except that MSTS input is case-insensitive) one of the names entered with the Rock or Soil Types card.

6.3.1 Mechanical Properties Card

Function

The Mechanical Properties card is used to assign values of porosity and tortuosity to rock or soil types identified with the Rock or Soil Types card.

Format

Line 0	"~Mechanical Properties"
Line 1	N { integer } " line(s) of mechanical properties input follows."
Line n	Rock or Soil Type { alpha (80 characters maximum) },
	Matrix Total Porosity n_T or n_{T_m} { real },
	Matrix Diffusive Porosity n_D or n_{D_m} { real },
	Matrix Effective Porosity n_E or n_{E_m} { real },
	Fracture Total Porosity n_{T_f} { real },
	Fracture Diffusive Porosity n_{D_f} { real },
	Fracture Effective Porosity n_{E_f} { real },
	Tortuosity variability option [constant | saturation dependent],
	Liquid Tortuosity τ_ℓ (not required for saturation-dependent option) { real },
	Gas Tortuosity τ_g (not required for saturation-dependent option) { real },

Comments

Mechanical properties are assigned by rock or soil type, which is input using the Rock or Soil Types card. The Rock or Soil Type field must contain a name that exactly matches one contained on the Rock or Soil Types card.

The (matrix) total, effective, and diffusive porosities must be specified for all rock or soil types named. The fracture porosities must be named only for rock or soil types for which the dual-porosity (equivalent-continuum) model is to be used.

Tortuosities can be specified under two options: "Constant" and "Saturation Dependent". If the Constant option is chosen, then a liquid-phase and/or gas-phase tortuosity must be specified. Zero values of tortuosity eliminate binary diffusion of gas-phase components and eliminate molecular diffusion for species transport. If the Saturation Dependent option is chosen, the liquid- and gas-phase tortuosities are computed from a model proposed by Millington and Quirk (1959), where the tortuosities are computed as a function of the porosity and phase saturation. Refer to Section 3.8 of the MSTS Theory Manual (White and Nichols 1992) for a model description.

Examples

In this example a single soil type, Yolo light clay, is assigned a total porosity of 0.495, an effective porosity of 0.371, and a diffusive porosity of 0.371. Only matrix flow is applicable to this soil type, so nothing is put between the three commas normally reserved for fracture porosities. The blank fields of tortuosity will result in constant tortuosities with zero value for both liquid and gas phases (i.e., no binary diffusion and no species diffusion transport).

```
~Mechanical Properties
1 line(s) of mechanical properties input follows.
Yolo Light Clay,0.495,0.371,0.371,,,,constant,,,
```

If the dual-porosity, equivalent-continuum approach is used for a rock type, then six porosity values are required. In this case, we specify two rock types, one that is fractured (Topopah Springs) and one that is not (Calico Hills). We also specify constant liquid and gas tortuosities:

```
~Mechanical Properties
2 line(s) of mechanical properties input follows.
Topopah Springs nonlithophysal,0.11,0.0088,0.11,0.43,0.0194,0.045,constant,0.02,0.20,
Calico Hills nonwelded zeolitic,0.28,0.2493,0.28,,,,constant,0.01,0.10,
```

6.3.2 Hydraulic Properties Card

Function

The Hydraulic Properties card is used to assign values of intrinsic permeability or hydraulic conductivity to rock or soil types identified with the Rock or Soil Types card.

Format

Line 0	"~Hydraulic Properties"
Line 1	N { integer } " line(s) of hydraulic properties input follows."
Line n	Rock or Soil Type { alpha (80 characters maximum) }, x- or r-Direction Matrix Intrinsic Permeability or Hydraulic Conductivity { real }, y- or θ-Direction Matrix Intrinsic Permeability or Hydraulic Conductivity { real }, z-Direction Matrix Intrinsic Permeability or Hydraulic Conductivity { real }, Units [m^2 | ft^2 | cm^2 | hc:m/s | hc:ft/s | hc:cm/s | hc:cm/day], x- or r-Direction Fracture Intrinsic Permeability or Hydraulic Conductivity { real }, y- or θ-Direction Fracture Intrinsic Permeability or Hydraulic Conductivity { real }, z-Direction Fracture Intrinsic Permeability or Hydraulic Conductivity { real }, Units [m^2 | ft^2 | cm^2 | hc:m/s | hc:ft/s | hc:cm/s | hc:cm/day], Coefficient of Specific Storage S_s { real }, Units [1/m | 1/ft | 1/cm],

Comments

Hydraulic properties are assigned by rock or soil type, which is input using the Rock or Soil Types card. The Rock or Soil Type field must contain a name that exactly matches one contained on the Rock or Soil Types card.

Enter values for fracture permeability (conductivity) only if you wish to invoke the equivalent-continuum, dual-porosity model (see Section 7.8 for details). Otherwise, enter only the matrix values and leave no characters between the commas for fracture values.

If only the water conservation equation is to be solved and it is preferable to enter hydraulic conductivity values rather than intrinsic permeability, precede the units with "hc:" to alert the MSTS code to this. For example, an isotropic hydraulic conductivity of 3.5 cm/s would be entered as:

```
~Hydraulic Properties
1 line(s) of hydraulic properties input follows.
Generic Sand,3.5,3.5,3.5,hc:cm/s,,,,,0.0,1/cm,
```

Hydraulic conductivity is converted to intrinsic permeability and storativity is converted to porous media compressibility internally in MSTS by assuming a reference temperature of 20°C. Notice that no fracture values were included in this example, so this material would be treated as a simple porous medium.

Examples

The following example provides input for a single rock or soil type, Yolo light clay, with an isotropic hydraulic conductivity of 1.23 x 10^{-7} m/s and a storativity of 0.124 1/m.

```
~Hydraulic Properties
1 line(s) of hydraulic properties input follows.
Yolo Light Clay,1.23e-7,1.23e-7,1.23e-7,hc:m/s,,,,hc:m/s,0.124,1/m,
```

If we entered the same properties using intrinsic permeabilities, the input card would look like this:

```
~Hydraulic Properties
1 line(s) of hydraulic properties input follows.
Yolo Light Clay,1.26E-14,1.26E-14,1.26E-14,m^2,,,,m^2,0.124,1/m,
```

The next example gives the parameters for a simulation that will use the equivalent-continuum, dual-porosity approach for one of two rock or soil types. The first layer is the Calico Hills nonwelded vitric, which has a saturated, isotropic hydraulic conductivity of 8.0 x 10^{-11} m/s and is not fractured. The second layer is the Topopah Springs welded nonlithophysal with a saturated, isotropic matrix hydraulic conductivity of 2.00 x 10^{-11} m/s and a saturated, isotropic fracture hydraulic conductivity of 8.3 x 10^{-5} m/s.

```
~Hydraulic Properties
2 line(s) of hydraulic properties input follows.
Calico Hills,8.0E-11,8.0E-11,8.0E-11,hc:m/s,,,,hc:m/s,0.0344,1/m,
Topopah Springs,2.0E-11,2.0E-11,2.0E-11,hc:m/s,8.3E-5,8.3E-5,8.3E-5,hc:m/s,0.0088,1/m,
```

6.3.3 Thermal Properties Card

Function

The Thermal Properties card is used to assign values of thermal conductivity, density, and specific heat to rock or soil types identified with the Rock or Soil Types card.

Format

Line 0	"~Thermal Properties"
Line 1	N { integer } " line(s) of thermal properties input follows."
Line n	Rock or Soil Type { alpha (80 characters maximum) },
	Effective Thermal Conductivity Model [dependent | independent | somerton]
	x- or r-Direction Unsaturated Thermal Conductivity { real },
	y- or θ-Direction Unsaturated Thermal Conductivity { real },
	z-Direction Unsaturated Thermal Conductivity { real },
	x- or r-Direction Saturated Thermal Conductivity { real },
	y- or θ-Direction Saturated Thermal Conductivity { real },
	z-Direction Saturated Thermal Conductivity { real },
	Units [W/m K | Btu/h ft F | cal/s cm K | Btu in/h ft^2 F],
	Rock or Soil Density ρ_s { real },
	Units [kg/m^3 | lbm/ft^3 | gm/cm^3],
	Rock or Soil Specific Heat c_s { real },
	Units [J/kg K | Btu/lbm F | cal/gm K],

Comments

Thermal properties are assigned by rock or soil type, which is input using the Rock or Soil Types card. The Rock or Soil Type field must contain a name that exactly matches one contained on the Rock or Soil Types card. The equivalent thermal conductivity of a partially saturated porous medium can be computed using three different models in MSTS. These models are described in Section 3.9 of the MSTS Theory Manual (White and Nichols 1992). The model choice is specified with the second option as "Independent," "Dependent," or "Somerton." The Dependent option combines a temperature-dependent liquid conductivity with an unsaturated solid thermal conductivity as a function of moisture content. The Independent option scales the saturated and unsaturated thermal conductivities with the liquid saturation. The Somerton option scales the saturated and unsaturated thermal conductivities with the square root of the liquid saturation.

Examples

The first example illustrates how to enter no thermal energy physical parameters at all for an isothermal simulation:

```
~Thermal Properties
0 line(s) of thermal properties input follows.
```

A problem with one rock or soil type of an isotropic material that has a thermal conductivity of 2.10 W/m K, a density of 2650 kg/m^3, and a specific heat of 1000 J/kg K would be entered as this example shows:

```
~Thermal Properties
1 line(s) of thermal properties input follows.
Generic Rock,dependent,2.10,2.10,2.10,,,,W/m K,2650,kg/m^3,1000,J/kg K,
```

If the same rock type were anisotropic, having a thermal conductivity twice as large in the vertical dimension as in the horizontal dimensions, the above example would be modified to appear as

```
~Thermal Properties
1 line(s) of thermal properties input follows.
Generic Rock,dependent,2.10,2.10,4.20,,,,W/m k,2650,kg/m^3,1000,J/kg K,
```

Finally, a three-rock domain could be defined with the following Thermal Properties card:

```
~Thermal Properties
3 line(s) of thermal properties input follows.
Rock Unit 1,dependent,1.0,1.0,2.0,,,,W/m K,2300,kg/m^3,1000,J/kg K,
Rock Unit 2,dependent,2.0,2.0,3.0,,,,W/m K,2400,kg/m^3,1050,J/kg K,
Rock Unit 3,dependent,3.0,3.0,4.0,,,,W/m K,2500,kg/m^3,1100,J/kg K,
```

6.3.4 Species Properties Card

Function

The Species Properties card is used to assign a species name and associated molecular diffusion coefficients, partition coefficients, and radioactive half-life to each rock or soil type identified with the Rock or Soil Types card. The current version of MSTS can simulate only one species at a time, but the species properties need to be identified with respect to each rock or soil type.

Format

Line 0	"~Species Properties"
Line 1	N { integer } " line(s) of species properties input follows."
Line n	Rock or Soil Type { alpha (80 characters maximum) },
	Species Name { alpha (80 characters maximum) },
	Liquid-Phase Molecular Diffusion Coefficient D_{d_ℓ} at 20°C and 1 atm { real },
	Units [m^2/s | ft^2/s | cm^2/s],
	Gas-Phase Molecular Diffusion Coefficient D_{d_g} at 20°C and 1 atm { real },
	Units [m^2/s | ft^2/s | cm^2/s],
	Liquid-Gas Partition Coefficient $K_{\ell g}$ { real },
	Units [cm^3 gas/gm liq. | liter gas/gm liq.],
	Solid-Liquid Partition Coefficient K_d { real },
	Units [gm liq./gm sol.],
	Species Half-Life $t_{1/2}$ { real },
	Units [s | min | h | day | wk | yr],

Comments

Species properties are indexed by rock or soil types because the molecular diffusion coefficients and phase partition coefficients may be dependent on the local geochemical environment. The Rock or Soil Type field must contain a name that exactly matches one contained on the Rock or Soil Types card. The liquid-gas partition coefficient equals the ratio of species concentration in the liquid phase to that in the gas phase. Similarly, the solid-liquid partition coefficient equals the ratio of the species concentration adsorbed on the solid phase to that dissolved in the liquid phase.

Examples

If the species mass conservation equation is not solved, the Species Properties card is entered

```
~Species Properties
0 line(s) of species properties input follows.
```

A simple example of species transport for a contaminant transported in liquid phase only through a single rock domain without retardation is

```
~Species Properties
1 line(s) of species properties input follows.
Generic Sand,Lead,1.0E-5,cm^2/s,,,,,,,,,
```

The following example illustrates the Species Properties card for ^{14}C, a radioactive isotope of carbon with a half-life of 5730 years, in a five-rock domain of volcanic tuffs. Carbon-14 is transported in both the liquid and the gas phases, so molecular diffusion and partition coefficients are all specified.

```
~Species Properties
5 line(s) of species properties input follows.
Welded,C14,1.77e-05,cm^2/s,0.152,cm^2/s,,carbon dioxide in water,0.0,gm liq./gm
       sol.,5730,yr,
Vitrophyre,C14,1.77e-05,cm^2/s,0.152,cm^2/s,,carbon dioxide in water,0.0,gm liq./gm
       sol.,5730,yr,
Vitric,C14,1.77e-05,cm^2/s,0.152,cm^2/s,,carbon dioxide in water,0.0,gm liq./gm
       sol.,5730,yr,
Zeolitic,C14,1.77e-05,cm^2/s,0.152,cm^2/s,,carbon dioxide in water,0.0,gm liq./gm
       sol.,5730,yr,
Partially Welded,C14,1.77e-05,cm^2/s,0.152,cm^2/s,,carbon dioxide in water,0.0,gm
       liq./gm sol.,5730,yr,
```

This example uses a special MSTS feature, "carbon dioxide in water," to describe the phase partition coefficients for the geochemical environment in the vadose zone at Yucca Mountain, Nevada.

6.3.5 Soil Characteristics Card

Function

The Soil Characteristics card is used to specify the relationship between liquid-gas capillary pressure and liquid saturation for unsaturated conditions for each rock or soil type identified on the Rock or Soil Types card. Several functions are available to express the soil-moisture-retention characteristics: van Genuchten, Brooks and Corey, Haverkamp, Leverett, or dual porosity with van Genuchten, as well as tabular input (see Section 7.0 for a description of these functions). The maximum tension head for each rock or soil type is also specified on this card.

Format

Line 0 "~Soil Characteristics"

Line 1: N { integer } " line(s) of soil characteristics input follows."

van Genuchten relation.

Line n
Rock or Soil Type { alpha (80 characters maximum) },
"van Genuchten,"
van Genuchten α Parameter { real },
Units [1/cm | 1/m | 1/ft],
van Genuchten n { real (dimensionless) },
Maximum Tension Head { real },
Units [m | ft | cm],
,
,

Brooks and Corey relation.

Line n
Rock or Soil Type { alpha (80 characters maximum) },
"Brooks and Corey,"
Brooks and Corey ψ^* parameter { real },
Units [cm | m | ft],
Brooks and Corey n parameter { real },
Maximum Tension Head { real },
Units [m | ft | cm],
,
,

Haverkamp relation.

Line n — Rock or Soil Type { alpha (80 characters maximum) },
"Haverkamp,"
Haverkamp α Parameter { real },
,
Haverkamp β { real (dimensionless) },
Maximum Tension Head { real },
Units [m | ft | cm],
,
,

Leverett relation.

Line n — Rock or Soil Type { alpha (80 characters maximum) },
"Leverett"
Residual Liquid Saturation s_ℓ { real },
,
Reference Capillary Pressure { real (Pa) },
Maximum Tension Head { real },
Units [m | ft | cm],
,
,

Dual-Porosity model.

Line n — Rock or Soil Type { alpha (80 characters maximum) },
"Dual Porosity,"
van Genuchten α_m Parameter for Matrix { real },
Units [1/cm | 1/m | 1/ft],
van Genuchten n_m Parameter for Matrix { real },
Maximum Tension Head { real },
Units [m | ft | cm],
van Genuchten α_f Parameter for Fracture { real },
Units [1/cm | 1/m | 1/ft]
van Genuchten n_f Parameter for Fracture{ real },

Tabular data.

Line n — Rock or Soil Type { alpha (80 characters maximum) },
"Tabular,"
"Table No. " M { integer },

Tables for tabular data follow all functional input lines. Tables must be ordered sequentially according to their respective table numbers.

Line 1 — N { integer} " line(s) of capillary tables input follows."

Line n — Tension Head ψ { real },
Liquid Saturation s_ℓ { real },
Tension Head Units [m | ft | cm],

Comments

Soil characteristics are assigned by rock or soil type, which is input using the Rock or Soil Types card. The Rock or Soil Type field must contain a name that exactly matches one contained on the Rock or Soil Types card. Functional specifications of the soil-moisture-retention functions are preferred over tabular descriptions.

Examples

One method to specify the relationship between liquid pressure and liquid saturation is to use tabular input. For example, suppose the Haverkamp relations (Haverkamp et al. 1977) were not available in MSTS to define the soil-moisture-retention characteristics of a soil and we wished to use that function with the following parameters: $\alpha = 200$, $\beta = 1.5$, $A = 100$, and $B = 2$. We could compute several pairs of tension head–liquid saturation points from the Haverkamp function (see Section 7.3 for the equation) and enter these as tabular input in the MSTS "input" file. Points on the soil-moisture-retention curve between tabular values are derived in MSTS by linear interpolation; hence, the greater the accuracy required, the greater the number of points should be in the tabular input that defines a nonlinear relationship such as this one. The resulting tabular input might appear as follows:

```
~Soil Characteristics
1 line(s) of soil characteristics input follows.
Generic Sand,Tabular,Table No. 1,
11 line(s) of capillary tables input follows.
0.1,0.9998,m,
1.0,0.995,m,
5,0.947,m,
10,0.863,m,
20,0.690,m,
40,0.441,m,
60,0.300,m,
80,0.218,m,
100,0.167,m,
1000,0.006,m,
10000,0.000,m,
```

If the parameters are available, functional relationships are preferred to tabular input because data entry is easier, the problems with linear interpolations are avoided, and solutions will be faster than for tabular input. In the following example, the van Genuchten relations are used to define soil characteristics for nine "zones," or rock types, as follows:

```
~Soil Characteristics
9 line(s) of soil characteristics input follows.
Zone 1,van Genuchten,.0456,1/cm,1.3661,1.0E+16,m,,,,
Zone 2,van Genuchten,.1109,1/cm,1.3428,1.0E+16,m,,,,
Zone 3,van Genuchten,.0427,1/cm,3.1603,1.0E+16,m,,,,
Zone 4,van Genuchten,.1533,1/cm,2.033,1.0E+16,m,,,,
Zone 5,van Genuchten,.0353,1/cm,2.8921,1.0E+16,m,,,,
Zone 6,van Genuchten,.0184,1/cm,3.3059,1.0E+16,m,,,,
Zone 7,van Genuchten,.0605,1/cm,2.4414,1.0E+16,m,,,,
Zone 8,van Genuchten,.0144,1/cm,5.4201,1.0E+16,m,,,,
Zone 9,van Genuchten,0.0810,1/cm,1.9709,1.0E+16,m,,,,
```

An example follows for the use of the Brooks and Corey function to define the soil-moisture-retention curve of sandy clay:

```
~Soil Characteristics
1 line(s) of soil characteristics input follows.
Sandy Clay,Brooks and Corey,32.75,cm,0.51,1.0E+12,m,,,
```

An example follows for the use of the Leverett function to define the soil-moisture-retention curve of sandy clay:

```
~Soil Characteristics
1 line(s) of soil characteristics input follows.
Zone 3,Leverett,0.05,,10132.0,1.0E+15,m,,,
```

6.3.6 Liquid Relative Permeability Card

Function

The Liquid Relative Permeability card is used to specify the liquid relative-permeability function for each rock or soil type identified on the Rock or Soil Types card. Several functions are available to express the relationship between liquid relative permeability and liquid saturation or between liquid relative permeability and capillary pressure head: Mualem pore distribution function integrated with the van Genuchten or Brooks and Corey soil-moisture-retention functions, Burdine pore distribution function integrated with the van Genuchten or Brooks and Corey soil-moisture-retention functions, Haverkamp function, Corey function, Fatt and Klikoff function, Touma and Vauclin function, or a dual-porosity model. Alternatively, tabular input may be used to define the relationship between liquid relative permeability and liquid saturation or between liquid relative permeability and capillary pressure head. The minimum liquid relative permeability for each rock or soil type is specified with the Liquid Relative Permeability card also.

Format

Line 0 "~Liquid Relative Permeability Properties"

Line 1 N { integer } " line(s) of liquid relative permeability input follows."

Mualem function with van Genuchten soil-moisture-retention relation.

Line n Rock or Soil Type { alpha (80 characters maximum) },
"Mualem w/ van Genuchten,"
van Genuchten m Parameter { real },
,
Minimum Liquid Relative Permeability { real },

Mualem function with Brooks and Corey soil-moisture-retention relation.

Line n Rock or Soil Type { alpha (80 characters maximum) },
"Mualem w/ Brooks & Corey,"
Brooks and Corey β Parameter { real },
,
Minimum Liquid Relative Permeability { real },

Burdine function with van Genuchten soil-moisture-retention relation.

Line n Rock or Soil Type { alpha (80 characters maximum) },
"Burdine w/ van Genuchten,"
van Genuchten m Parameter { real },
,
Minimum Liquid Relative Permeability { real },

Burdine function with Brooks and Corey soil-moisture-retention relation.

Line n Rock or Soil Type { alpha (80 characters maximum) },
"Burdine w/ Brooks & Corey,"
Brooks and Corey β Parameter { real },
,
Minimum Liquid Relative Permeability { real },

Haverkamp relation.

Line n Rock or Soil Type { alpha (80 characters maximum) },
"Haverkamp,"
Haverkamp A Parameter { real },
Haverkamp B Parameter { real },
Minimum Liquid Relative Permeability { real },

Corey relation.

Line n Rock or Soil Type { alpha (80 characters maximum) },
"Corey's Curves,"
Residual Liquid Saturation s_ℓ { real },
Entrapped Air Saturation $s_{\ell s}$ { real },
Minimum Liquid Relative Permeability { real },

Fatt and Klikoff relation.

Line n Rock or Soil Type { alpha (80 characters maximum) },
"Fatt and Klikoff"
Residual Liquid Saturation $s_{\ell r}$ { real },
,
Minimum Liquid Relative Permeability { real },

Touma and Vauclin relation.

Line n Rock or Soil Type { alpha (80 characters maximum) },
"Touma and Vauclin"
Fitting Parameter A_ℓ { real },
Fitting Parameter B_ℓ { real },
Minimum Liquid Relative Permeability { real },

Dual-porosity model.

Line n Rock or Soil Type { alpha (80 characters maximum) },
"Dual Porosity"
van Genuchten m_m Parameter for Matrix { real },
,
Minimum Liquid Relative Permeability { real },
van Genuchten m_f Parameter for Fracture { real },

Tabular versus Liquid Saturation.

Line n Rock or Soil Type { alpha (80 characters maximum) },
"Tabular vs Liquid Saturation,"
"Table No. " M { integer },

Tables for tabular data follow all functional input lines. Tables must be ordered sequentially according to their respective table numbers.

Line 1 N { integer } " line(s) of liquid permeability tables input follows."

Line n Liquid Saturation s_ℓ { real },
Liquid Relative Permeability $k_{r\ell}$ { real },

Tabular versus Tension Head.

Line n Rock or Soil Type { alpha (80 characters maximum) },
"Tabular vs Tension Head,"
"Table No. " M { integer },

Tables for tabular data follow all functional input lines. Tables must be ordered sequentially according to their respective table numbers.

Line 1 N { integer } " line(s) of liquid permeability tables input follows."

Line n Tension Head ψ { real },
Liquid Relative Permeability $k_{r\ell}$ { real },
Tension Head Units [m | ft | cm],

Comments

Liquid relative permeabilities are assigned by rock or soil type, which is input using the Rock or Soil Types card. The Rock or Soil Type field must contain a name that exactly matches one contained on the Rock or Soil Types card. Functional specifications of the liquid relative-permeability functions are preferred over tabular descriptions. For additional details on the various functional relationships (e.g., Mualem, Burdine) available with this card, refer to Section 7.0.

Examples

Tabular input is the most difficult to enter into MSTS input files, so the first two examples illustrate this type of specification for liquid relative permeability. The first example shows a tabular form of the liquid relative-permeability function proposed by Haverkamp et al. (1977), in the form of liquid relative permeability versus liquid saturation, as follows:

```
~Liquid Relative Permeability Properties
1 line(s) of liquid relative permeability input follows.
Generic Sand,Tabular vs Liquid Saturation,Table No. 1,
11 line(s) of liquid permeability tables input follows.
1.000,1.000,
0.998,0.998,
0.947,0.800,
0.863,0.500,
0.691,0.200,
0.442,0.059,
0.301,0.027,
0.218,0.015,
0.167,0.010,
0.006,9.99E-5,
0.000,1.00E-6,
```

Alternatively, we can define the liquid relative permeability as a function of tension head, as follows:

```
~Liquid Relative Permeability Properties
1 line(s) of liquid relative permeability input follows.
Generic Sand,Tabular vs Tension Head,Table No. 1,
12 line(s) of liquid permeability tables input follows.
0.00,1.00,m,
0.1,0.999,m,
1.0,0.990,m,
5.0,0.800,m,
10.0,0.500,m,
20.0,0.200,m,
40.0,0.059,m,
60.0,0.027,m,
80.0,0.015,m,
100.0,0.010,m,
1000.0,1.00E-6,m,
10000.0,1.00E-6,m,
```

Notice in both tabular examples that the endpoints of the curves are established at zero capillary pressure ($s_\ell = 1.0$) and at the minimum relative conductivity for the problem (1.0×10^{-6} m in this case); this practice serves to avoid undefined regions of these relationships.

Functional relations are easier to enter than tabular input. An example of the liquid relative-permeability function specified using the Corey function appears as follows:

```
~Liquid Relative Permeability Properties
1 line(s) of liquid relative permeability input follows.
Generic Sand,Corey's Curves,0.30,0.05,1.0E-10,,
```

In this example, the minimum relative liquid permeability is 1.0×10^{-10}, the parameter residual liquid saturation equals 0.30, and the entrapped air at saturation equals 0.05. See Section 7.0 for details on the parameters used in Corey's Curves and other relative-permeability functions.

The final example of liquid relative-permeability input is for a seven-rock-type problem where some of the rock types are fractured and use the dual-porosity model while others are not

fractured and use Mualem functions with van Genuchten soil-moisture-retention relations.

```
~Liquid Relative Permeability Properties
7 line(s) of liquid relative permeability input follows.
Nonwelded Ash Flow,Mualem w/ van Genuchten,0.3333,,1.0e-12,,
Bedded Tuff,Mualem w/ van Genuchten,0.900,,1.0e-12,,
Welded Nonlithophysal,Dual Porosity,0.4438,,1.0e-12,0.6269,
Vitrophyre,Dual Porosity,0.4438,,1.0e-12,0.6269,
Vitric,Dual Porosity,0.5502,,1.0e-12,0.6269,
Zeolitic,Dual Porosity,0.1909,,1.0e-12,0.6269,
Partially Welded,Dual Porosity,0.6212,,1.0e-12,0.6269,
```

6.3.7 Gas Relative Permeability Card

Function

The Gas Relative Permeability card is used to specify the gas permeability function for each rock or soil type identified on the Rock or Soil Types card. Several functions are available to express the relationship between gas relative permeability and liquid saturation or between gas relative permeability and capillary pressure head: Corey function, Fatt and Klikoff function, Touma and Vauclin function, or a linear relationship with the liquid relative permeability of the same rock or soil type. Alternatively, tabular input may be used to define the relationship between gas relative permeability and liquid saturation or between gas relative permeability and capillary pressure head. The minimum gas relative permeability for each rock or soil type is also specified with the Gas Relative Permeability card.

Format

Line 0 "~Gas Relative Permeability Properties"

Line 1 N { integer } " line(s) of gas relative permeability input follows."

Corey relation.

Line n Rock or Soil Type { alpha (80 characters maximum) },
"Corey's Curves,"
Residual Liquid Saturation $s_{\ell r}$ { real },
Entrapped Air Saturation $s_{\ell s}$ { real },
Minimum Gas Relative Permeability { real },

Fatt and Klikoff relation.

Line n Rock or Soil Type { alpha (80 characters maximum) },
"Fatt and Klikoff"
Residual Liquid Saturation $s_{\ell r}$ { real },
,
Minimum Gas Relative Permeability { real },

Touma and Vauclin relation.

Line n Rock or Soil Type { alpha (80 characters maximum) },
"Touma and Vauclin"
Fitting Parameter A_g { real },
Fitting Parameter B_g { real },
Minimum Gas Relative Permeability { real },

Linear with liquid relative permeability.

Line n Rock or Soil Type { alpha (80 characters maximum) },
"Linear w/ Liq. Rel. Perm.,"

Tabular versus Liquid Saturation.

Line n Rock or Soil Type { alpha (80 characters maximum) },
"Tabular vs Liquid Saturation,"
"Table No. " M { integer },

Tables for tabular data follow all functional input lines. Tables must be ordered sequentially according to their respective table numbers.

Line 1 N { integer } " line(s) of gas permeability tables input follows."

Line n Liquid Saturation s_ℓ { real },
Gas Relative Permeability k_{rg} { real },

Tabular versus Tension Head.

Line n Rock or Soil Type { alpha (80 characters maximum) },
"Tabular vs Tension Head,"
"Table No. " M { integer },

Tables for tabular data follow all functional input lines. Tables must be ordered sequentially according to their respective table numbers.

Line 1 N { integer} " line(s) of gas permeability tables input follows."

Line n Tension Head ψ { real },
Gas Relative Permeability k_{rg} { real },
Tension Head Units [m | ft | cm],

Comments

Gas relative permeabilities are assigned by rock or soil type, which is input using the Rock or Soil Types card. The Rock or Soil Type field must contain a name that exactly matches one contained on the Rock or Soil Types card. Functional specifications of the gas relative-permeability functions are preferred over tabular descriptions. For additional details on the various functional relationships (e.g., Corey, Fatt and Klikoff) available with this card, refer to Section 7.0.

Examples

As with liquid permeability relations, tabular input for gas permeability relations is the most complex type of entry. This example illustrates how to make gas relative permeability vary linearly with liquid saturation using tabular input for a single-rock-type problem:

```
~Gas Relative Permeability Properties
1 line(s) of gas relative permeability input follows.
Generic Sand,Tabular vs Liquid Saturation,Table No. 1,
2 line(s) of gas permeability tables input follows.
0.0,1.0,
1.0,1.0,
```

Gas relative permeability can be expressed in terms of tension head (liquid-gas capillary pressure head), as well as liquid saturation. Of course, nonlinear relationships require more than two data points to adequately define a curve.

Another option for gas relative permeability is to relate it linearly to liquid relative permeability, as for this clay problem:

```
~Gas Relative Permeability Properties
1 line(s) of gas relative permeability input follows.
Yolo Light Clay,Linear w/ Liq. Rel. Perm.,
```

The method used to define gas relative permeability can be different for different rock or soil types as well. Here, one rock type is described by a Fatt and Klikoff relation while a second is described by tabular input as a function of liquid saturation.

```
~Gas Relative Permeability Properties
2 line(s) of gas relative permeability input follows.
Sample,Fatt and Klikoff,0.15,,1.0E-06,
Slick Rock,Tabular vs Liquid Saturation,Table No. 2,
3 line(s) of gas permeability tables input follows.
0.0,0.4286,
0.15,0.4286,
1.0,0.4286,
```

6.4 Boundary Conditions

Boundary conditions are specified through five distinct boundary condition cards: liquid, gas, vapor, thermal energy, and species. The Liquid Boundary Conditions card specifies boundary conditions for aqueous pressure, aqueous component mass fractions, aqueous density, and aqueous fluxes. The Gas Boundary Conditions card specifies boundary conditions for gas pressure, gas component mass fractions, gas density, and gas fluxes. The Vapor Boundary Condition card specifies boundary conditions only with respect to diffusion of components through the gas phase; the advection of components in the gas phase at boundary surfaces is specified through the gas boundary conditions. Having unique boundary conditions for the advection and diffusion transport mechanisms for gas components allows greater flexibility in creating problem definitions. For example, this approach allows the user to simulate boundaries that are impermeable to advective flow but permit gas component diffusion. The Energy Boundary Conditions card specifies boundary conditions for temperature, volumetric enthalpies for liquid and gas, and heat fluxes. The Species Boundary Conditions card specifies boundary conditions for species concentrations in the aqueous and gas phases and species boundary surface fluxes individually for the aqueous- and gas-phase fluxes. The default boundary condition for every undeclared boundary surface is a zero-flux condition for liquid-phase mass, gas-phase mass, vapor diffusion, heat, and species mass.

6.4.1 Liquid Boundary Conditions Card

Function

The Liquid Boundary Conditions card is used to specify boundary conditions for aqueous pressure, aqueous component mass fractions, aqueous density, and aqueous fluxes at the external boundaries of the problem domain and at the boundaries of inactive nodes. Four boundary condition types are available: Dirichlet, Neumann, saturated, and unit gradient.

Format

Line 0 "~Liquid Boundary Conditions"

Line 1 N { integer } " line(s) of liquid boundary conditions input follows."

Dirichlet Boundary.

Line n
Direction [X-Direction | Y-Direction | Z-Direction]:
Surface [Top | Bottom | East | West | North | South] " Surface,"
"Dirichlet @ Boundary,"
Liquid Pressure P_ℓ { real },
Units [Pa (absolute) | Psi (absolute) | Atm (absolute) | Bar (absolute)],
Liquid Density ρ_ℓ { real },
Units [kg/m^3 | lbm/ft^3 | gm/cm^3],
Air Mass Fraction x_ℓ^a { real },
I Start { integer },
I End { integer },
J Start { integer },
J End { integer },
K Start { integer },
K End { integer },

Neumann Boundary.

Line n
Direction [X-Direction | Y-Direction | Z-Direction]:
Surface [Top | Bottom | East | West | North | South] " Surface,"
"Neumann @ Boundary,"
Liquid Mass Flux $\dot{Q}_\ell$ { real },
Units [kg/m^2 s | lbm/ft^2 s | gm/cm^2 s],
,
,
Air Mass Fraction x_ℓ^a { real },
I Start { integer },
I End { integer },
J Start { integer },
J End { integer },
K Start { integer },
K End { integer },

Saturated Boundary.

Line n Direction [X-Direction | Y-Direction | Z-Direction]:
Surface [Top | Bottom | East | West | North | South] " Surface,"
"Saturated @ Boundary,"
,
,
Liquid Density ρ_ℓ { real },
Units [kg/m^3 | lbm/ft^3 | gm/cm^3],
Air Mass Fraction x_ℓ^a { real },
I Start { integer },
I End { integer },
J Start { integer },
J End { integer },
K Start { integer },
K End { integer },

Unit-Gradient Boundary.

Line n Direction [X-Direction | Y-Direction | Z-Direction]:
Surface [Top | Bottom | East | West | North | South] " Surface,"
"Unit Gradient @ Boundary,"
,
,
Liquid Density ρ_ℓ { real },
Units [kg/m^3 | lbm/ft^3 | gm/cm^3],
Air Mass Fraction x_ℓ^a { real },
I Start { integer },
I End { integer },
J Start { integer },
J End { integer },
K Start { integer },
K End { integer },

Comments

Boundary conditions must be applied to active nodes adjacent to exterior boundary surfaces or inactive nodes. The surface orientations refer to a boundary surface with respect to the active node. Dirichlet-type boundary conditions are used to specify liquid pressures at a boundary surface. The phase density and component mass fractions will be used for boundary surface mass fluxes that are directed into the active node. Neumann-type boundary conditions are used to specify liquid-phase mass fluxes at a boundary surface. Flux directions are aligned with the coordinate directions. A positive flux in the x- or r-direction is toward the east, in the y- or θ-direction is toward the north, and in the z-direction is toward the top. Saturated boundary conditions maintain a zero capillary pressure head at the boundary surface (i.e., liquid pressure is

maintained equal to the gas pressure). Unit-gradient-type boundary conditions are used to specify surface fluxes at the boundary that result from gravitational body forces only. Unit-gradient-type boundary conditions applied to vertical surfaces are equivalent to zero-flux boundary conditions.

Examples

A one-dimensional problem requires boundaries to be defined only at the ends of the problem, because the default boundary conditions for undeclared surfaces are zero-flux boundaries. Here a one-dimensional, vertically oriented problem is assigned a constant liquid mass flux in the negative *z*-direction (the sign of the flux indicates direction) into the domain at the top of the porous medium column and a constant saturation condition (water table) at the bottom.

```
~Liquid Boundary Conditions
2 line(s) of liquid boundary conditions input follows.
Z-Direction: Top Surface,Neumann @ Boundary,-2.0,kg/m^2 s,,,0,1,1,1,1,9,9,
Z-Direction: Bottom Surface,Saturated @ Boundary,,,998.3,kg/m^3,,1,1,1,1,1,1,
```

6.4.2 Gas Boundary Conditions Card

Function

The Gas Boundary Conditions card is used to specify boundary conditions for gas pressure, gas component mass fractions, gas density, and gas fluxes at the external boundaries of the problem domain and at the boundaries of inactive nodes. Three boundary condition types are available: Dirichlet, Neumann, and unit gradient.

Format

Line 0 "~Gas Boundary Conditions"

Line 1 N { integer } " line(s) of gas boundary conditions input follows."

Dirichlet Boundary.

Line n
Direction [X-Direction | Y-Direction | Z-Direction]:
Surface [Top | Bottom | East | West | North | South] " Surface,"
"Dirichlet @ Boundary,"
Gas Pressure P_g { real },
Units [Pa (absolute) | Psi (absolute) | Atm (absolute) | Bar (absolute)],
Gas Density ρ_g { real },
Units [kg/m^3 | lbm/ft^3 | gm/cm^3],
Water-Vapor Mass Fraction x_g^w { real },
I Start { integer },
I End { integer },
J Start { integer },
J End { integer },
K Start { integer },
K End { integer },

Neumann Boundary.

Line n
Direction [X-Direction | Y-Direction | Z-Direction]:
Surface [Top | Bottom | East | West | North | South] " Surface,"
"Neumann @ Boundary,"
Gas Mass Flux $\dot{Q}_g$ { real },
Units [kg/m^2 s | lbm/ft^2 s | gm/cm^2 s],
,
,
Water-Vapor Mass Fraction x_g^w { real },
I Start { integer },
I End { integer },
J Start { integer },
J End { integer },
K Start { integer },
K End { integer },

Unit-Gradient Boundary.

Line n Direction [X-Direction | Y-Direction | Z-Direction]:
Surface [Top | Bottom | East | West | North | South] " Surface,"
"Unit Gradient @ Boundary,"
,
,
Gas Density ρ_g { real },
Units [kg/m^3 | lbm/ft^3 | gm/cm^3],
Water-Vapor Mass Fraction x_g^w { real },
I Start { integer },
I End { integer },
J Start { integer },
J End { integer },
K Start { integer },
K End { integer },

Comments

Boundary conditions must be applied to active nodes adjacent to exterior boundary surfaces or inactive nodes. The surface orientations refer to a boundary surface with respect to the active node. Dirichlet-type boundary conditions are used to specify gas pressures at a boundary surface. The phase density and component mass fractions will be used for boundary surface mass fluxes that are directed into the active node. Neumann-type boundary conditions are used to specify gas-phase mass fluxes at a boundary surface. Flux directions are aligned with the coordinate directions. A positive flux in the x- or r-direction is toward the east, in the y- or θ-direction is toward the north, and in the z-direction is toward the top. Unit-gradient-type boundary conditions are used to specify surface fluxes at the boundary that result from gravitational body forces only. Unit-gradient-type boundary conditions applied to vertical surfaces are equivalent to zero-flux boundary conditions.

Examples

The first example is for a problem that does not require a gas boundary condition to be defined:

```
~Gas Boundary Conditions
0 line(s) of gas boundary conditions input follows.
```

A common gas boundary condition is constant atmospheric pressure. Here, a Dirichlet boundary is defined on the west surface of a problem domain with constant gas pressure of 101,330 Pa, gas density at this boundary of 0.91944 kg/m^3, and vapor mass fraction 0.21395:

```
~Gas Boundary Conditions
1 line(s) of gas boundary conditions input follows.
X-Direction: West Surface,Dirichlet @ Boundary,101330.0,Pa
        (absolute),0.91944,kg/m^3,0.21395,1,1,1,1,1,1,
```

6.4.3 Vapor Boundary Conditions Card

Function

The Vapor Boundary Conditions card specifies boundary conditions only with respect to diffusion of components through the gas phase; the advection of components in the gas phase at boundary surfaces is specified through gas boundary conditions. Vapor boundary conditions can be declared at the external boundary surfaces of the problem domain and at the boundaries between active and inactive nodes. Only Dirichlet-type boundary conditions are available for vapor boundary conditions.

Format

Line 0 "~Vapor Boundary Conditions"

Line 1 N { integer } " line(s) of vapor boundary conditions input follows."

Dirichlet Boundary.

Line n Direction [X-Direction | Y-Direction | Z-Direction]:
Surface [Top | Bottom | East | West | North | South] " Surface,"
"Dirichlet @ Boundary,"
Water-Vapor Mass Fraction x_g^w { real },
I Start { integer },
I End { integer },
J Start { integer },
J End { integer },
K Start { integer },
K End { integer },

Comments

Boundary conditions must be applied to active nodes adjacent to exterior boundary surfaces or inactive nodes. The surface orientations refer to a boundary surface with respect to the active node. Dirichlet-type boundary conditions are used to specify water-vapor mass fraction at a boundary surface. Water-vapor mass fractions declared through the Vapor Boundary Conditions card are used only to compute the diffusion of water vapor across a boundary surface. Advection of water vapor across a boundary surface is controlled through the Gas Boundary Conditions card. Normally, the water-vapor mass fractions declared on the Vapor Boundary Conditions and Gas Boundary Conditions cards will be equivalent.

Examples

If no vapor boundary conditions are to be declared in an "input" file, the Vapor Boundary Conditions card would be entered as

```
~Vapor Boundary Conditions
0 line(s) of vapor boundary conditions input follows.
```

In the next example, the Vapor Boundary Conditions card is provided for a model domain with an upper boundary that is the interface with the atmosphere. The upper boundary is a sloping surface, so inactive nodes (refer to Section 6.2.2 for information on inactive node declaration) are used to represent the atmosphere, and the boundary is defined at the edge of the inactive region. The vapor boundary condition in this example is a constant vapor mass fraction of 0.003.

```
~Vapor Boundary Conditions
21 line(s) of vapor boundary conditions input follows.
Z-Direction: Top Surface,Dirichlet @ Boundary,0.003,1,1,1,1,50,50,
Z-Direction: Top Surface,Dirichlet @ Boundary,0.003,2,4,1,1,49,49,
Z-Direction: Top Surface,Dirichlet @ Boundary,0.003,5,8,1,1,48,48,
Z-Direction: Top Surface,Dirichlet @ Boundary,0.003,9,11,1,1,47,47,
Z-Direction: Top Surface,Dirichlet @ Boundary,0.003,12,14,1,1,46,46,
Z-Direction: Top Surface,Dirichlet @ Boundary,0.003,15,17,1,1,45,45,
Z-Direction: Top Surface,Dirichlet @ Boundary,0.003,18,21,1,1,44,44,
Z-Direction: Top Surface,Dirichlet @ Boundary,0.003,22,24,1,1,43,43,
Z-Direction: Top Surface,Dirichlet @ Boundary,0.003,25,27,1,1,42,42,
Z-Direction: Top Surface,Dirichlet @ Boundary,0.003,28,30,1,1,41,41,
Z-Direction: Top Surface,Dirichlet @ Boundary,0.003,31,34,1,1,40,40,
Z-Direction: Top Surface,Dirichlet @ Boundary,0.003,35,37,1,1,39,39,
Z-Direction: Top Surface,Dirichlet @ Boundary,0.003,38,40,1,1,38,38,
Z-Direction: Top Surface,Dirichlet @ Boundary,0.003,41,42,1,1,37,37,
Z-Direction: Top Surface,Dirichlet @ Boundary,0.003,43,47,1,1,36,36,
Z-Direction: Top Surface,Dirichlet @ Boundary,0.003,48,54,1,1,35,35,
Z-Direction: Top Surface,Dirichlet @ Boundary,0.003,55,60,1,1,34,34,
Z-Direction: Top Surface,Dirichlet @ Boundary,0.003,61,67,1,1,33,33,
Z-Direction: Top Surface,Dirichlet @ Boundary,0.003,68,73,1,1,32,32,
Z-Direction: Top Surface,Dirichlet @ Boundary,0.003,74,83,1,1,31,31,
Z-Direction: Top Surface,Dirichlet @ Boundary,0.003,84,91,1,1,30,30,
```

6.4.4 Energy Boundary Conditions Card

Function

The Energy Boundary Conditions card specifies boundary conditions for temperature, volumetric enthalpies for liquid and gas, and heat fluxes at the external boundaries of the problem domain and at the boundaries of inactive nodes (if any). Two boundary condition types are available: Dirichlet and Neumann.

Format

Line 0 "~Energy Boundary Conditions"

Line 1 N { integer } " line(s) of energy boundary conditions input follows."

Dirichlet Boundary.

Line n
Direction [X-Direction | Y-Direction | Z-Direction]:
Surface [Top | Bottom | East | West | North | South] " Surface,"
"Dirichlet @ Boundary,"
Temperature T { real },
Units [Celsius | Fahrenheit | Rankine | Kelvin],
Liquid Volumetric Enthalpy h_ℓ { real },
Units [J/m^3 | Btu/ft^3 | cal/cm^3],
Gas Volumetric Enthalpy h_g { real },
Units [J/m^3 | Btu/ft^3 | cal/cm^3],
I Start { integer },
I End { integer },
J Start { integer },
J End { integer },
K Start { integer },
K End { integer },

Neumann Boundary.

Line n Direction [X-Direction | Y-Direction | Z-Direction]:
Surface [Top | Bottom | East | West | North | South] " Surface,"
"Neumann @ Boundary,"
Heat Flux $\dot{Q}_{e,n}$ { real },
Units [W/m^2 | Btu/h ft^2 | cal/cm^2 s],
Liquid Volumetric Enthalpy h_ℓ { real },
Units [J/m^3 | Btu/ft^3 | cal/cm^3],
Gas Volumetric Enthalpy h_g { real },
Units [J/m^3 | Btu/ft^3 | cal/cm^3],
I Start { integer },
I End { integer },
J Start { integer },
J End { integer },
K Start { integer },
K End { integer },

Comments

Boundary conditions must be applied to active nodes adjacent to exterior boundary surfaces or inactive nodes. The surface orientations refer to a boundary surface with respect to the active node. Dirichlet-type boundary conditions are used to specify temperatures at a boundary surface. The liquid and gas volumetric enthalpies will be used for boundary surface mass fluxes that are directed into the active node. Neumann-type boundary conditions are used to specify heat fluxes at a boundary surface. Flux directions are aligned with the coordinate directions. A positive flux in the x- or r-direction is toward the east, in the y- or θ-direction is toward the north, and in the z-direction is toward the top.

Examples

These are the boundary conditions for a one-dimensional, horizontally oriented heat pipe problem (see Section 8.0 for a complete description of the heat pipe problem). The east side is assigned a constant energy flux of 100 W/m^2 directed into the domain (the negative sign indicates the direction of the flux) while the west side is assigned a constant temperature of 70°C.

```
~Energy Boundary Conditions
2 line(s) of energy boundary conditions input follows.
X-Direction: West Surface,Dirichlet @ Boundary,70,Celsius,2.864e+8,J/m^3,5.2098e+5,
       J/m^3,1,1,1,1,1,1,
X-Direction: East Surface,Neumann @ Boundary,-100,W/m^2,,J/m^3,,J/m^3,50,50,1,1,1,1,
```

Any boundary condition can be applied either to the domain boundary or to the surface of inactive nodes (see Section 6.2.2 for information on declaring inactive nodes). In the following example of an Energy Boundary Conditions card, a boundary at a constant temperature of 20°C is assigned to the top of a two-dimensional (*x*-*z*), 5 by 5 node domain that has inactive nodes in the lower left-hand side. A constant temperature of 30°C is assigned to the top of each inactive node that is adjacent to a computational node to form a diagonal boundary in the problem.

```
~Energy Boundary Conditions
5 line(s) of energy boundary conditions input follows.
Z-Direction: Top Surface,Dirichlet @ Boundary,20.,Celsius,8.379e+07,J/m^3,2.e+04,
       J/m^3,1,5,1,1,5,5,
Z-Direction: Bottom Surface,Dirichlet @ Boundary,30.,Celsius,1.252e+08,J/m^3,0.,
       J/m^3,4,5,1,1,1,1,
Z-Direction: Bottom Surface,Dirichlet @ Boundary,30.,Celsius,1.252e+08,J/m^3,0.,
       J/m^3,3,3,1,1,2,2,
Z-Direction: Bottom Surface,Dirichlet @ Boundary,30.,Celsius,1.252e+08,J/m^3,0.,
       J/m^3,2,2,1,1,3,3,
Z-Direction: Bottom Surface,Dirichlet @ Boundary,30.,Celsius,1.252e+08,J/m^3,0.,
       J/m^3,1,1,1,1,4,4,
```

6.4.5 Species Boundary Conditions Card

Function

The Species Boundary Conditions card specifies boundary conditions for species concentrations in the aqueous and gas phases and species boundary surface fluxes individually for the aqueous- and gas-phase fluxes at the external boundaries of the problem domain and at the boundaries of inactive nodes. Two boundary condition types are available: Dirichlet and Neumann.

Format

Line 0 "~Species Boundary Conditions"

Line 1 N { integer } " line(s) of species boundary conditions input follows."

Dirichlet Boundary.

Line n
Direction [X-Direction | Y-Direction | Z-Direction]:
Surface [Top | Bottom | East | West | North | South] " Surface,"
"Dirichlet @ Boundary,"
Liquid-Phase Species Concentration C_ℓ { real },
Units [(mol;Ci)/m^3 | (mol;Ci)/ft^3 | (mol;Ci)/liter | (mol;Ci)/cm^3)],
Gas-Phase Species Concentration C_g { real },
Units [(mol;Ci)/m^3 | (mol;Ci)/ft^3 | (mol;Ci)/liter | (mol;Ci)/cm^3)],
I Start { integer },
I End { integer },
J Start { integer },
J End { integer },
K Start { integer },
K End { integer },

Neumann Boundary.

Line n
Direction [X-Direction | Y-Direction | Z-Direction]:
Surface [Top | Bottom | East | West | North | South] " Surface,"
"Neumann @ Boundary,"
Liquid-Phase Species Flux $\dot{Q}_{c_\ell}$ { real },
Units [(mol;Ci)/m^2 s | (mol;Ci)/ft^2 s |(mol;Ci)/cm^2 s)],
Gas-Phase Species Flux $\dot{Q}_{c_g}$ { real },
Units [(mol;Ci)/m^2 s | (mol;Ci)/ft^2 s |(mol;Ci)/cm^2 s)],
I Start { integer },
I End { integer },
J Start { integer },
J End { integer },
K Start { integer },
K End { integer },

Comments

Boundary conditions must be applied to active nodes adjacent to exterior boundary surfaces or inactive nodes. The surface orientations refer to a boundary surface with respect to the active node. Dirichlet-type boundary conditions are used to specify species concentrations at a boundary surface. Neumann-type boundary conditions are used to specify species fluxes at a boundary surface. Flux directions are aligned with the coordinate directions. A positive flux in the x- or r-direction is toward the east, in the y- or θ-direction is toward the north, and in the z-direction is toward the top.

Examples

A two-dimensional, horizontally oriented, 75-node transport problem with constant concentrations at each end (1.0 mol/liter at the west side, 0.1 mol/liter at the east side) is entered as

```
~Species Boundary Conditions
2 line(s) of species boundary conditions input follows.
X-Direction: West Surface,Dirichlet @ Boundary,1.0,(mol;ci)/liter,,,1,1,1,1,1,1,
X-Direction: East Surface,Dirichlet @ Boundary,0.1,(mol;ci)/liter,,,75,75,1,1,1,1,
```

If default boundary conditions (zero-flux) are desired, or the species transport equation is not activated, then the Species Boundary Conditions card is entered as

```
~Species Boundary Conditions
0 line(s) of species boundary conditions input follows.
```

6.5 Initial Conditions and Sources

The initial conditions for a simulation problem can be specified either through a "restart" file or with the Initial Conditions card. When the initial conditions are specified with a "restart" file, information on the Initial Conditions card is ignored. The Initial Conditions card allows users to specify values for the primary variables and Darcy velocities, when appropriate. For added flexibility, the Initial Conditions card provides three methods for specifying the liquid pressure, gas pressure, and liquid saturation. Because the soil-moisture-retention functions relate these variables, only two of three variables are required to completely specify the hydrologic state of the system. For example, the user may specify the liquid saturation and gas pressure on the Initial Conditions card, and the corresponding liquid pressure field would be computed internally by MSTS. Alternatively, the gas pressure and liquid pressure could be specified and MSTS would compute the corresponding liquid saturation.

The Sources and Sinks card is used to define sources or sinks for water mass, air mass, thermal energy, and species mass or concentration. Sources may be defined as constant for a certain time period or may vary following a table of values as a function of time. Each source is defined with respect to a rectangular range of source node(s), though multiple Sources and Sinks cards can be used to give geometric flexibility in defining a source.

6.5.1 Initial Conditions Card

Function

The Initial Conditions card is used to specify the values of field variables at computational nodes at the start of a simulation (time zero). No primary variable initial conditions are required for restart simulations. Field variables are defined at node points, whereas field velocities or fluxes are defined on node surfaces. The field velocity associated with a particular node index is defined for the lower surface (e.g., west, south, bottom). For example, *x*-direction velocities defined at a node with (I, J, K) indices refers to the *x*-direction velocity at the west surface of the node with the same indices. Uncomputed velocity variables must be specified for both normal and restart simulations. The Initial Saturation option declares which two variables among the liquid pressure, gas pressure, and liquid saturation will be used to specify the initial hydrologic conditions.

Format

Line 0 "~Initial Conditions"

Line 1 Initial Saturation [Liquid Saturation & Gas Pressure | Liquid Saturation & Liquid Pressure | Gas Pressure & Liquid Pressure]

Line 2 N { integer } " line(s) of initial conditions input follows."

Line n Field Variable Name [Liquid Pressure | Gas Pressure | Liquid Saturation | Temperature | Species Concentration | X–Dir. Liquid Velocity | Y–Dir. Liquid Velocity | Z–Dir. Liquid Velocity | X–Dir. Gas Velocity | Y–Dir. Gas Velocity | Z–Dir. Gas Velocity | Vapor Mass Fraction],
Field Variable Value { real },
Units *Pressure.* [Pa (absolute) | Psi (absolute) | Atm (absolute) | Bar (absolute)],
Saturation. (dimensionless),
Temperature. [Celsius | Fahrenheit | Rankine | Kelvin],
Concentration. [(mol;ci)/m^3 | (mol;ci)/ft^3 | (mol;ci)/liter | (mol;ci)/cm^3]
Velocity. [m/s | ft/s | cm/s | m/h | ft/h | cm/h | m/day | ft/day | cm/day],
Vapor Mass Fraction. (dimensionless),
x-Direction Gradient { real },
Units [1/m | 1/ft | 1/cm],
y-Direction Gradient { real },
Units [1/m | 1/ft | 1/cm],
z-Direction Gradient { real },
Units [1/m | 1/ft | 1/cm],
I Start { integer },
I End { integer },
J Start { integer },
J End { integer },
K Start { integer },
K End { integer },

Comments

Unless the simulation is beginning from a "restart" file, primary variable initial conditions must be specified. Default initial conditions for the primary variables are the following: liquid pressure (101325 Pa), gas pressure (101325 Pa), temperature (20 °C), and species concentration (0 mol/m^3). Default initial conditions for the secondary variables are the following: liquid saturation (0 m^3/m^3) and vapor mass fraction (thermodynamic saturation conditions for two-phase conditions, 0 kg/kg for gas-phase-only conditions). Default initial conditions for Darcy velocities are 0 m/s. Before being used in MSTS, initial conditions are checked for thermodynamic consistency and operational limits. The following restrictions apply to the primary variable initial conditions: liquid pressure (611.25 Pa $\leq P_\ell \leq$ 2.212 x 10^7 Pa), gas pressure (611.25 Pa $\leq P_g \leq$ 2.212 x 10^7 Pa), temperature (0.01°C $\leq T \leq$ 374.14°C). Thermodynamic consistency checks are performed on two-phase nodes for evaporation and on gas-phase-only nodes for condensation. To satisfy thermodynamic equilibrium conditions for two-phase nodes (i.e., nodes with both liquid and gas phases present), the specified gas pressure must be greater than the saturated water-vapor partial pressure. To satisfy thermodynamic equilibrium conditions for gas-phase-only nodes (i.e., nodes with only the gas phase present), the specified vapor mass fraction must be less than the saturated vapor mass fraction. If either of these conditions is violated, the simulation is aborted, with an error message printed to the "output" file.

Initial species concentrations are expressed in terms of the total volume, rather than gas- or aqueous-phase volumes. For example, initial concentrations expressed per unit aqueous-phase volume must be converted to concentrations per unit total volume by multiplying the aqueous-phase concentration by the product of the diffusive porosity (n_D) and the liquid saturation under initial conditions (s_ℓ).

To simplify the specification of initial conditions, the Initial Conditions card accepts initial conditions expressed in terms of linear gradients. Gradients are expressed in terms of dimensional length and start at the node position of the node indexed on the Initial Conditions card. An excellent example of specifying initial conditions in terms of gradients results from the specification of an initial liquid saturation field under static equilibrium conditions. For a simulation involving the Water mode, specifying a constant gradient to the liquid pressure field that decreases with elevation by the product of the aqueous-phase density and acceleration of gravity (–9793.5 Pa/m @ 20°C) will result in an initial liquid saturation field at static equilibrium. The water table height for such initial conditions will be located at the point of zero capillary pressure.

Examples

The initial condition for a 100-node vertically oriented, one-dimensional problem is atmospheric gas pressure and a liquid pressure of 42000 Pa (absolute) throughout. The Initial Conditions card for this case appears as

```
~Initial Conditions
Gas Pressure & Liquid Pressure,
2 line(s) of initial conditions input follows.
Gas Pressure,101325.0,Pa (absolute),0.0,1/m,0.0,1/m,0.0,1/m,1,1,1,1,1,100,
Liquid Pressure,42000.0,Pa (absolute),0.0,1/m,0.0,1/m,0.0,1/m,1,1,1,1,1,100,
```

The initial condition is not restricted to a single value for the whole problem domain. One way to vary the condition is by specifying different values for different ranges of nodes. For example, the previous card can be modified to give the same liquid pressure at time zero for the lower half of the nodes, but a lower pressure for the upper half:

```
~Initial Conditions
Gas Pressure & Liquid Pressure,
3 line(s) of initial conditions input follows.
Gas Pressure,101325.0,Pa (absolute),0.0,1/m,0.0,1/m,0.0,1/m,1,1,1,1,1,100,
Liquid Pressure,42000.0,Pa (absolute),0.0,1/m,0.0,1/m,0.0,1/m,1,1,1,1,1,50,
Liquid Pressure,21000.0,Pa (absolute),0.0,1/m,0.0,1/m,0.0,1/m,1,1,1,1,51,100,
```

If a uniform variation of initial conditions is desired, use the gradient utility. For example, if the initial conditions of a one-dimensional, 10-m-long, horizontally oriented problem, with a uniform grid, vary linearly from zero liquid saturation at the left side to fully saturated at the right side, the initial condition could be specified as

```
~Initial Conditions
Gas Pressure & Liquid Saturation,
2 line(s) of initial conditions input follows.
Gas Pressure,101325.0,Pa (absolute),0.0,1/m,0.0,1/m,0.0,1/m,1,50,1,1,1,1,
Liquid Saturation,0.01,,0.1,1/m,0.0,1/m,0.0,1/m,1,50,1,1,1,1,
```

which would cause the initial condition of zero saturation at the west boundary to be increased 0.1 per meter until reaching 1.0 (fully saturated) at 10 m, which is the east boundary. The gradient feature may be used with any initial condition in any dimension(s).

6.5.2 Sources and Sinks Card

Function

The Sources and Sinks card is used to identify the location and strength of sources and/or sinks of liquid mass, air mass, thermal energy, and species mass. The strength of a source or sink either may be constant in time or may vary following tabular input.

Format

Line 0	"~Sources & Sinks"
Line 1	N { integer } " line(s) of sources & sinks input follows."
Line n	Source Type [Liquid Mass | Gas Mass | Thermal Energy | Species | Species Concentration],

Liquid Mass.

Source Variation [Constant | Tabular],

Constant.

Liquid Mass Source Rate $\dot{m}_\ell$ { real },
Units [kg/s | lbm/s | gm/s | kg/h | lbm/h | gm/h | kg/day | lbm/day | gm/day],
Liquid Enthalpy h_ℓ { real },
Units [J/kg | Btu/lbm | cal/gm],
Air Mass Fraction x_ℓ^a { real },
Source Start Time { real },
Units [s | min | h | day | wk | yr],
Source End Time { real },
Units [s | min | h | day | wk | yr],
I Start { integer },
I End { integer },
J Start { integer },
J End { integer },
K Start { integer },
K End { integer },

Tabular.

Table Number { integer },
,
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,
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,
,
,
,
I Start { integer },
I End { integer },
J Start { integer },
J End { integer },
K Start { integer },
K End { integer },

Line n M { integer } " line(s) of source tables input follows."

Line m Time { real },
Units [s | min | h | day | wk | yr],
Liquid Mass Source Rate $\dot{m}_\ell$ { real },
Units [kg/s | lbm/s | gm/s | kg/h | lbm/h | gm/h | kg/day | lbm/day | gm/day],
Liquid Enthalpy h_ℓ { real },
Units [J/kg | Btu/lbm | cal/gm],
Air Mass Fraction { real },

Gas Mass.

Source Variation [Constant | Tabular],

Constant.

Gas Mass Source Rate $\dot{m}_g$ { real },
Units [kg/s | lbm/s | gm/s | kg/h | lbm/h | gm/h | kg/day | lbm/day | gm/day],
Gas Enthalpy h_g { real },
Units [J/kg | Btu/lbm | cal/gm],
Vapor Mass Fraction x_g^w { real },
Source Start Time { real },
Units [s | min | h | day | wk | yr],
Source End Time { real },
Units [s | min | h | day | wk | yr],
I Start { integer },
I End { integer },
J Start { integer },
J End { integer },
K Start { integer },
K End { integer },

Tabular.

Table Number { integer },
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I Start { integer },
I End { integer },
J Start { integer },
J End { integer },
K Start { integer },
K End { integer },

Line n M { integer } " line(s) of source tables input follows."

Line m Time { real },
Units [s | min | h | day | wk | yr],
Gas Mass Source Rate $\dot{m}_g$ { real },
Units [kg/s | lbm/s | gm/s | kg/h | lbm/h | gm/h | kg/day | lbm/day | gm/day],
Gas Enthalpy h_g { real },
Units [J/kg | Btu/lbm | cal/gm],
Vapor Mass Fraction { real },

Thermal Energy.

Source Variation [Constant | Tabular],

Constant.

Energy Source Rate $\dot{Q}$ { real },
Units [W/m^3 | Btu/h ft^3 | cal/s cm^3],
,
,
,
,
Source Start Time { real },
Units [s | min | h | day | wk | yr],
Source End Time { real },
Units [s | min | h | day | wk | yr],
I Start { integer },
I End { integer },
J Start { integer },
J End { integer },
K Start { integer },
K End { integer },

Tabular.

Table Number { integer },
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,
I Start { integer },
I End { integer },
J Start { integer },
J End { integer },
K Start { integer },
K End { integer },

Line n M { integer } " line(s) of source tables input follows."

Line m Time { real },
Units [s | min | h | day | wk | yr],
Energy Source Rate { real },
Units [W/m^3 | Btu/h ft^3 | cal/s cm^3],
,
,
,

Species.

Source Variation [Constant | Tabular],

Constant.

Species Mass Source Rate $\dot{s}_c$ { real },
[(mol;Ci)/s | (mol;Ci)/h | (mol;Ci)/day],
,
,
,
Source Start Time { real },
Units [s | min | h | day | wk | yr],
Source End Time { real },
Units [s | min | h | day | wk | yr],
I Start { integer },
I End { integer },
J Start { integer },
J End { integer },
K Start { integer },
K End { integer },

Tabular.

Table Number { integer },
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I Start { integer },
I End { integer },
J Start { integer },
J End { integer },
K Start { integer },
K End { integer },

Line n M { integer } " line(s) of source tables input follows."

Line m Time { real },
Units [s | min | h | day | wk | yr],
Species Mass Source Rate $\dot{s}_c$ { real },
[(mol;Ci)/s | (mol;Ci)/h | (mol;Ci)/day],
,
,
,

Species Concentration.

Source Variation [Constant | Tabular],

Constant.

Species Mass Concentration Source Rate $\dot{s}_{c,v}$ { real },
[(mol;Ci)/m^3 s | (mol;Ci)/m^3 h | (mol;Ci)/m^3 day],
,
,
,
Source Start Time { real },
Units [s | min | h | day | wk | yr],
Source End Time { real },
Units [s | min | h | day | wk | yr],
I Start { integer },
I End { integer },
J Start { integer },
J End { integer },
K Start { integer },
K End { integer },

Tabular.

Table Number { integer },
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,
I Start { integer },
I End { integer },
J Start { integer },
J End { integer },
K Start { integer },
K End { integer },

Line n M { integer } " line(s) of source tables input follows."

Line m Time { real },
Units [s | min | h | day | wk | yr],
Species Mass Concentration Source Rate $\dot{s}_c$ { real },
[(mol;Ci)/m^3 s | (mol;Ci)/m^3 h | (mol;Ci)/m^3 day],
,
,
,

Comments

The source quantity (liquid mass, gas mass, thermal energy, or species mass) is per grid cell over the range of grid nodes identified by the I Start, I End, J Start, J End, K Start, and K End integer fields. Therefore, if 1.0 kg/s of liquid mass is the source for the range of nodes (1,3,1,1,1,1), then a total of 3.0 kg/s of mass will be introduced to the problem domain. Source term rates between tabular inputs are obtained with linear interpolation; therefore, the integrated source quantity will be dependent on the simulation time step. Strongly varying source terms will require smaller time steps to accurately model the integrated source quantity.

Enthalpy inputs associated with the liquid and gas mass sources are used only if the solution option includes an active energy equation. If the energy equation is inactive (i.e., unsolved), then these values are unused and blank entries may be used. Enthalpy inputs include both water and air components for the gas phase, but only water components for the liquid phase. Component enthalpies are combined by mass fraction weighting. The reference point for water enthalpy is liquid water at 0.01°C whereas the reference point for air enthalpy is gaseous air at 0°C.

Species "mass" may represent either the number of moles of the substance (e.g., mol/s represents the number of moles introduced per second) or the activity of a radionuclide, expressed in curies (Ci). Input and output are marked in both units (e.g., mol;Ci/s). The actual unit is based on the use of the code, so that if the input reflects activity, so does the output.

Species sources may be expressed as either concentration per unit time or mass per unit time. Sources expressed as concentration per unit time are usually preferred for source regions comprising several grid nodes of varying size, because MSTS will introduce a mass source equally to nodes regardless of cell volume. This would result in artificial concentration variation due purely to cell volume. This is not a problem if all grid cells in the source region (defined by I Start, I End, J Start, J End, K Start, and K End) are the same volume or if only one node is defined as a source region.

Examples

A problem that has no internal sources or sinks will have a Sources and Sinks card that appears as

```
~Sources & Sinks
0 line(s) of sources & sinks input follows.
```

The following example is for a problem with a time-varying source that releases nothing at time zero and increases the release by an additional 1.0 Ci/m^3 s each year for a period of 5 years. The time variation of the source is expressed in tabular input (Table 1).

```
~Sources & Sinks
1 line(s) of sources & sinks input follows.
Species Concentration,Tabular,1,,,,,,,,,1,4,1,1,21,21,
6 line(s) of source tables input to follow.
0.00E+00,yr,0.00E+00,(mol;ci)/m^3 s,,,,,
1.00E+00,yr,1.00E+00,(mol;ci)/m^3 s,,,,,
2.00E+00,yr,2.00E+00,(mol;ci)/m^3 s,,,,,
3.00E+00,yr,3.00E+00,(mol;ci)/m^3 s,,,,,
4.00E+00,yr,4.00E+00,(mol;ci)/m^3 s,,,,,
5.00E+00,yr,5.00E+00,(mol;ci)/m^3 s,,,,,
```

A thermal-energy source of 20,000 W/m^3 that is constant from time zero to 1875 seconds for a single grid node might look like the last example:

```
~Sources & Sinks
1 line(s) of sources & sinks input follows.
Thermal Energy,Constant,2.0E+5,W/m^3,,,,,0,s,1875.0,s,1,1,1,1,1,1,
```

6.6 Output Control

Output control occurs in MSTS using the Liquid Pathline Trace card, Output Control card, and Surface Flux Integrator card. The Liquid Pathline Trace card invokes an algorithm for groundwater travel time that is based on the mean velocity of water though the model domain. The starting coordinates of a pathline are defined along with the circumstances under which to cease a trace, such as reaching a certain plane or crossing a specified distance. The Output Control card is used to indicate precisely what field variables should be recorded at what times and over what range of computational nodes. Separate output can be requested for the "output" and "plot" files, and for reference node reporting during a simulation execution. The Surface Flux Integrator card is useful for obtaining the flux of liquid mass, gas mass, species mass or concentration, or energy across specified planes.

6.6.1 Liquid Pathline Trace Card

Function

The Liquid Pathline Trace card is used to define pathline beginning locations and termination conditions to be traced by MSTS to produce the pathline geometry and characteristic travel times based on mean liquid velocities.

Format

Line 0	"~Liquid Pathline Trace"
Line 1	N { integer } " line(s) of liquid pathline trace input follows."
Line n	Pathline Identification Number { integer }, Start Time { real }, Units [s | min | h | day | wk | yr], Initial x- or r-Direction Coordinate { real }, Units [m | ft | cm], Initial y- or θ-Direction Coordinate { real }, Units [m | ft | cm], Initial z-Direction Coordinate { real }, Units [m | ft | cm], Termination Condition [Boundary | Saturation | X | Y | Z], Termination-Plane Index { integer },

Comments

The pathline identification number is purely for differentiating between pathlines. The identification numbers do not need to be in strictly increasing order or follow other restrictions.

The boundary termination condition directs MSTS to trace a pathline until the pathline encounters a problem domain boundary (including boundaries represented by internal nodes) or the end of the simulation. This is the default termination condition.

A saturation termination condition may be used only for pathlines that begin in an unsaturated region. The pathline is traced until fully saturated conditions are encountered, a grid boundary is reached, or the simulation ends.

The termination-plane conditions (X, Y, and Z) are used to force MSTS to stop tracing a pathline when a particular X, Y, or Z plane is encountered and record the travel time. If this condition is used, the value of the index of the surface plane must also be provided. The termination-plane associated with a particular node index is defined for the lower cell surface (e.g., west, south, bottom).

Examples

Here three pathlines are defined for travel time calculations in a two-dimensional (x-z) unsaturated domain problem. All three are initially at the top of the domain (z = 10 m). The first pathline will be traced until a boundary is encountered. The second will be traced until it reaches the water table at the bottom of the problem domain or a boundary. The third will terminate when (and if) it encounters the point half-way down at z = 5 m. All are started at time zero.

```
~Liquid Pathline Trace
3 line(s) of liquid pathline trace input follows.
1,0.0,yr,1.0,m,1.0,m,10.0,m,Boundary,,
2,0.0,yr,2.0,m,0.0,m,10.0,m,Saturation,,
3,0.0,yr,3.0,m,0.0,m,10.0,m,Z,5.0,
```

6.6.2 Output Control Card

Function

The Output Control card is used to specify conventional output, plotting output, and reference nodes output. Output controlled through this card is recorded on the "output" file, the "plot" file, and the output screen. Conventional output, which includes input records, simulation process data, reference node data, and field variable data is recorded on the "output" file. Plotting output, which contains condensed formats of field data, is recorded on the "plot" file. Reference nodes output, which includes selected field variables data for a maximum of four nodes is recorded both on the "output" file and output screen. Output times, structures, and formats are also controlled with the Output Control card. The "output" file contains records of specified field variables over a specified domain, presented as two-dimensional arrays of information. Conversely, the "plot" file contains records of specified field variables for every node (including inactive nodes), ordered sequentially by node number. Node numbers are ordered in the sequence row, column, tier, where rows represent east-west directions, columns represent north-south directions, and tiers represent top-bottom directions.

Format

Line 0	"~Output Control"
Line 1	Field Variable Domain ("output" file) I Start { integer }, Field Variable Domain ("output" file) I End{ integer }, Field Variable Domain ("output" file) J Start { integer }, Field Variable Domain ("output" file) J End { integer }, Field Variable Domain ("output" file) K Start { integer }, Field Variable Domain ("output" file) K End { integer }, Plane [xyplane | yzplane | zxplane | yxplane | zyplane | xzplane],
Line 2	N { integer } " line(s) of output control input follows."
Line n	Field Variable Output Time ("output" file and "plot" file) { real }, Units [s | min | h | day | wk | yr],
Next Line	Reference Node 1 I-index { integer }, Reference Node 1 J-index { integer }, Reference Node 1 K-index { integer }, Reference Node 2 I-index { integer }, Reference Node 2 J-index { integer }, Reference Node 2 K-index { integer }, Reference Node 3 I-index { integer }, Reference Node 3 J-index { integer }, Reference Node 3 K-index { integer }, Reference Node 4 I-index { integer },

	Reference Node 4 J-index { integer },
	Reference Node 4 K-index { integer },
	Reference Node Output Frequency (Time Steps per Output){ integer },
Next Line	N { integer } " line(s) of output control input follows."
Line n	{"output" file field variable- see Table 6.3 for acceptable field variable names},
Next Line	N { integer } " line(s) of output control input follows."
Line n	{"plot" file field variable- see Table 6.3 for acceptable field variable names},
Next Line	N { integer } " line(s) of output control input follows."
Line n	{reference node field variable- see Table 6.3 for acceptable field variable names},

Comments

Because of line width restrictions on computer screens, a maximum of seven field variables may be selected for reference node output. Although there is no limit to the number of field variables that may be selected for "output" file and "plot" file output, the number of selected field variables should be limited to maintain conveniently sized files. The output field velocities associated with a particular node index are defined for the lower surface (e.g., west, south, bottom). For example, an x-direction velocity defined at a particular node with (I, J, K) indices refers to the x-direction velocity at the west surface of the node with the same indices.

Table 6.3. MSTS Field Variables Available for"Output" File,"Plot" File, and Reference Node Records

Field Variable	Name Used in Output Control Card
P_ℓ	Liquid Pressure
P_g	Gas Pressure
T	Temperature
C	Species Concentration
s_ℓ	Liquid Saturation
s_g	Gas Saturation
x_ℓ^a	Liquid Phase Air Mass Fraction
x_g^a	Gas Phase Vapor Mass Fraction
$k_{r\ell}$	Liquid Phase Relative Permeability
k_{rg}	Gas Phase Relative Permeability
ρ_ℓ	Liquid Density
ρ_g	Gas Density
H_T	Total Hydraulic Head
θ	Volumetric Moisture Content
χ_ℓ^a	Species Liquid Phase Mole Fraction
χ_g^a	Species Gas Phase Mole Fraction
V_ℓ	X-Direction Liquid Velocity
V_ℓ	Y-Direction Liquid Velocity
V_ℓ	Z-Direction Liquid Velocity
V_g	X-Direction Gas Velocity
V_g	Y-Direction Gas Velocity
V_g	Z-Direction Gas Velocity
$\dot{Q}_{e,\gamma}$	X-Direction Heat Transfer Rate

Table 6.3. (Contd)

Field Variable	Name Used in Output Control Card
$\dot{Q}_{e,\gamma}$	Y-Direction Heat Transfer Rate
$\dot{Q}_{e,\gamma}$	Z-Direction Heat Transfer Rate
$\dot{Q}_{c,\gamma}$	X-Direction Species Flux
$\dot{Q}_{c,\gamma}$	Y-Direction Species Flux
$\dot{Q}_{c,\gamma}$	Z-Direction Species Flux

Examples

Careful use of the Output Control card will yield output to meet the user's needs without swamping files and computer monitors with undesired information. Here is an example of an Output Control card:

```
~Output Control
1,91,1,1,1,50,zxplane,
4 line(s) of output control input follows.
4000,yr,
6000,yr,
8000,yr,
10000,yr,
1,1,21,66,1,21,1,1,50,66,1,33,1,
0 line(s) of output control input follows.
1 line(s) of output control input follows.
Species Concentration,
5 line(s) of output control input follows.
Liquid Pressure,
Gas Pressure,
Temperature,
Species Concentration,
Liquid Saturation,
```

In the example, MSTS output is specified for the region between nodes 1 and 91 in the x- or r-direction, nodes 1 and 1 in the y- or θ-direction, and nodes 1 and 50 in the z-direction. Output is requested at four simulation times: 4000, 6000, 8000, and 10,000 years. Four reference nodes are designated at node positions (1,1,21), (66,1,21), (1,1,50), and (66,1,33). No field variables will be output to "output" file. Only species concentration will be recorded to the "plot" file. Five field variables will be displayed on the computer monitor during the simulation for the reference nodes: liquid pressure, gas pressure, temperature, species concentration, and liquid saturation.

6.6.3 Surface Flux Integrator Card

Function

The Surface Flux Integrator card is use to specify two-dimensional planes across which fluxes of liquid mass, gas mass, thermal energy, and species mass are recorded and integrated after each simulation time step. Surface orientation is with respect to an active node.

Format

Line 0 "~Surface Flux Integrator"

Line 1 N { integer } " line(s) of surface flux integrator input follows."

Line n Surface Orientation [X-Direction: West Surface | X-Direction: East Surface | Y-Direction: South Surface | Y-Direction: North Surface | Z-Direction: Bottom Surface | Z-Direction: Top Surface],
Surface Flux Type [Liquid Phase | Gas Phase | Thermal Energy | Species Concentration],
I Start { integer },
I End { integer },
J Start { integer },
J End { integer },
K Start { integer },
K End { integer },

Comments

The surface flux integrator serves several purposes. For example, the surface flux integrator feature can be used to test for steady-state conditions by comparing influx and outflow of a quantity at domain boundaries. More commonly, the surface flux integrator is used to determine the flux of a contaminant or the heat transfer across an outflow boundary as a function of simulation time. The surface flux integrator considers the diffusive, advective, and dispersive components of flux. The release of a radionuclide to the water table from an unsaturated model with a saturated lower boundary condition is an example of this use.

Examples

If no surface flux integration is desired, enter the following for the Surface Flux Integrator card:

```
~Surface Flux Integrator
0 line(s) of surface flux integrator input follows.
```

The following input card could be used to obtain a record of water flux entering and leaving a one-dimensional, vertically oriented, 50-node problem in which the water direction is downward:

```
~Surface Flux Integrator
2 line(s) of surface flux integrator input follows.
Z-Direction: Top Surface,Liquid Phase,1,1,1,1,50,50,
Z-Direction: Bottom Surface,Liquid Phase,1,1,1,1,1,1,
```

7.0 Water-Retention and Relative-Permeability Functions

A number of functional relations are available for use in MSTS to define the water-retention and relative-permeability characteristics of a porous medium. The available functions are defined in this section for reference.

7.1 van Genuchten Relations

The van Genuchten (1980) relations are available in MSTS for defining water-retention and liquid relative-permeability functions. For this functional description, effective liquid saturation (s_ℓ^*) is defined as

$$s_\ell^* = \frac{s_\ell - s_{\ell r}}{1 - s_{\ell r}} \tag{7.1}$$

where s_ℓ is the liquid saturation and $s_{\ell r}$ is the residual liquid saturation, with the restriction $0 \le s_{\ell r} \le s_\ell \le 1$. The effective liquid saturation is expressed as a function of tension head (ψ) in the following manner:

$$s_\ell^* = \left[1 + (\alpha\psi)^n\right]^{-m} \qquad \psi < 0 \tag{7.2a}$$

$$s_\ell^* = 1 \qquad \psi \ge 0 \tag{7.2b}$$

where α and n are empirically determined van Genuchten fitting parameters (α has the dimension L^{-1} and n is dimensionless) and m is a function of n:

$$m = 1 - \frac{1}{n} \tag{7.2c}$$

The equation used to compute liquid relative permeability under the van Genuchten relations depends on whether the formula of Burdine (1953) or Mualem (1976) is chosen. If Burdine's equation is specified, the liquid relative hydraulic conductivity ($k_{r\ell}$) under unsaturated conditions is expressed as

$$k_{r\ell}(s_\ell^*) = (s_\ell^*)\, 2\left[1 - \left(1 - (s_\ell^*)^{\frac{1}{m}}\right)^m\right] \tag{7.3}$$

but if Mualem's equation is specified, then the expression for $k_{r\ell}$ is

$$k_{r\ell}(s_\ell^*) = (s_\ell^*)^{\frac{1}{2}}\left[1 - \left(1 - (s_\ell^*)^{\frac{1}{m}}\right)^m\right]^2 \tag{7.4}$$

Section 6.3.6 (Liquid Relative Permeability Card) indicates how to specify Mualem's or Burdine's formula in MSTS input.

7.2 Brooks and Corey Relations

The Brooks and Corey relations are available in MSTS for defining water-retention and liquid relative-permeability functions. For this functional description, effective liquid saturation (s_ℓ^*) is defined as

$$s_\ell^* = \frac{s_\ell - s_{\ell r}}{1 - s_{\ell r}} \tag{7.5}$$

where s_ℓ is the liquid saturation and $s_{\ell r}$ is the residual liquid saturation, with the restriction $0 \le s_{\ell r} \le s_\ell \le 1$. The effective liquid saturation is expressed as a function of tension head (ψ) in the following manner:

$$s_\ell^* = \left(\frac{\psi}{\psi^*}\right)^{-m} \qquad \psi < \psi^* \tag{7.6a}$$

$$s_\ell^* = 1 \qquad \psi \ge \psi^* \tag{7.6b}$$

where ψ^* is the air-entry head (minimum drainage capillary pressure at which a continuous nonwetting phase exists) and m is an empirical constant. The constant m is a measure of the pore-size distribution of the media.

The liquid relative-permeability function depends on whether Burdine (1953) or Mualem (1976) relations are specified. If Burdine relations are chosen, then liquid relative permeability ($k_{r\ell}$) is computed from

$$k_{r\ell}(s_\ell^*) = s_\ell^{*\left(3 + \frac{2}{m}\right)} \tag{7.7}$$

while if Mualem relations are chosen, the equation used is

$$k_{r\ell}(s_\ell^*) = s_\ell^{*\left(\frac{5}{2} + \frac{2}{m}\right)} \tag{7.8}$$

Section 6.3.6 (Liquid Relative Permeability Card) indicates how to specify Mualem's or Burdine's formula in MSTS input.

7.3 Haverkamp Relations

The Haverkamp relations (Haverkamp et al. 1977) are available in MSTS for defining water-retention and liquid relative-permeability functions. For this functional description, effective liquid saturation (s_ℓ^*) is defined as

$$s_\ell^* = \frac{s_\ell - s_{\ell r}}{1 - s_{\ell r}} \tag{7.9}$$

where s_ℓ is the liquid saturation and $s_{\ell r}$ is the residual liquid saturation, with the restriction $0 \le s_{\ell r} \le s_\ell \le 1$. The effective liquid saturation is expressed as a function of tension head (ψ) in the following manner:

$$s_\ell^* = \frac{\alpha}{\alpha + (\ln|100\,\psi|)^\beta} \qquad \psi < 0 \tag{7.10a}$$

$$s_\ell^* = 1 \qquad \psi \ge 0 \tag{7.10b}$$

where α and β are curve-fitting parameters and tension head is expressed in meters. The liquid relative permeability ($k_{r\ell}$) is computed from

$$k_{r\ell} = \frac{A}{A + (100\,\psi)^B} \tag{7.11}$$

where A and B are curve-fitting parameters and tension head is again expressed in meters.

7.4 Corey Relations

Corey's Curves are available in MSTS for defining water-retention, liquid relative-permeability, and gas relative-permeability functions. For this functional description, effective liquid saturation (s_ℓ^*) is defined as

$$s_\ell^* = \frac{s_\ell - s_{\ell r}}{1 - s_{\ell r} - s_{sr}} \tag{7.12}$$

where s_ℓ is the liquid saturation, $s_{\ell r}$ is the residual liquid saturation, and s_{sr} is the entrapped air

saturation with the restriction that $(s_{\ell r} + s_{sr}) < 1$. The relative liquid permeability ($k_{r\ell}$) is

$$k_{r\ell} = \left(s_\ell^*\right)^4 \tag{7.13}$$

and the relative gas permeability (k_{rg}) is

$$k_{rg} = \left(1 - s_\ell^*\right)^2 \left[1 - \left(s_\ell^*\right)^2\right] \tag{7.14}$$

7.5 Fatt and Klikoff Relations

The relations of Fatt and Klikoff (1959) are available in MSTS for defining water-retention, liquid relative-permeability, and gas relative-permeability functions. For this functional description, effective liquid saturation (s_ℓ^*) is defined as

$$s_\ell^* = \frac{s_\ell - s_{\ell r}}{1 - s_{\ell r}} \tag{7.15}$$

where s_ℓ is the liquid saturation and $s_{\ell r}$ is the liquid residual saturation with the restriction $0 \le s_{\ell r} \le s_\ell \le 1$. Liquid relative permeability ($k_{r\ell}$) is computed as

$$k_{r\ell} = \left(s_\ell^*\right)^3 \tag{7.16}$$

and gas relative permeability (k_{rg}) is expressed as

$$k_{rg} = \left(1 - s_\ell^*\right)^3 \tag{7.17}$$

7.6 Leverett Relations

Leverett's function (Leverett 1941; Udell and Fitch 1985) is available in MSTS for defining water-retention, liquid relative-permeability, and gas relative-permeability functions. For this functional description, effective liquid saturation (s_ℓ^*) is defined as

$$s_\ell^* = \frac{s_\ell - s_{\ell r}}{1 - s_{\ell r}} \tag{7.18}$$

with the restriction that $0 \le s_{\ell r} \le s_\ell \le 1$. The capillary pressure (P_{cap}) is computed from

$$P_g - P_\ell = -P_{cap}^* \, \sigma^{aw} f \tag{7.19}$$

where σ^{aw} is the surface tension of water (supplied internally by MSTS as a function of temperature) and f is computed from

$$f = 1.417\left(1 - s_\ell^*\right) - 2.120\left(1 - s_\ell^*\right)^2 + 1.263\left(1 - s_\ell^*\right)^3 \tag{7.20}$$

7.7 Touma and Vauclin Relations

Touma and Vauclin (1986) used, for modeling purposes, analytical expressions fitted to experimental data to describe the dependence of liquid and gas relative permeabilities on liquid saturation. The MSTS form of their expression to describe liquid relative permeability as function of volumetric moisture content θ is

$$k_{r\ell} = A_\ell \, \theta^{B_\ell} \tag{7.21}$$

where A_ℓ and B_ℓ are empirical fitting parameters. The gas relative permeability is expressed as a function of the capillary pressure head, or tension head ψ:

$$k_{rg} = \frac{A_g}{A_g + \psi^{B_g}} \tag{7.22}$$

where A_g and B_g are empirical fitting parameters. This function was introduced to MSTS for the explicit purpose of simulating problems for Section 8.6 (One-Dimensional Two-Phase Infiltration).

7.8 Dual-Porosity Model With van Genuchten Relations

An equivalent-continuum (dual-porosity) model is available in MSTS to define water-retention and liquid relative-permeability functions. The model represents a composite domain that includes the effects of both fracture- and matrix-flow regimes. The equivalent bulk aqueous saturation (s_{ℓ_b}) is approximated as

$$s_{\ell_b} = \frac{s_{\ell_f} n_{T_f} + s_{\ell_m}\left(1 - n_{T_f}\right) n_{T_m}}{n_{T_f} + \left(1 - n_{T_f}\right) n_{T_m}} \tag{7.23}$$

where s_{ℓ_f} is the liquid saturation of the fractures, s_{ℓ_m} is the liquid saturation of the matrix, n_{T_f} is the total porosity of the fractures (ratio of the fracture volume to the total bulk volume), and n_{T_m} is

the total porosity of the matrix (ratio of the volume of the voids in the matrix to the total bulk volume). The equivalent bulk aqueous relative permeability ($k_{r\ell_b}$) is defined as

$$k_{r\ell_b} = k_{r\ell_m}\left(1 - n_{T_f}\right) + k_{r\ell_f} n_{T_f} \tag{7.24}$$

where $k_{r\ell_f}$ and $k_{r\ell_m}$ are the fracture and matrix relative liquid permeabilities, respectively.

8.0 Sample Problems

Eight sample problems are presented in this section. The sample problems were selected to demonstrate the application of MSTS to a variety of thermal and hydrogeologic transport problems. The eight sample problems are summarized in Table 8.1 and include single-phase flow and transport, multiphase flow and heat transfer, interphase mass transfer, and phase transition. The sample problems demonstrate the application of the code's various solution modes and provide complete examples of MSTS input files. Sample problem results are compared to analytical, semi-analytical, independent numerical, and experimental results.

In all of these sample problems, the input files for the MSTS code used to direct the simulations described in each section (and in some cases the output files) are shown as "exhibits." Each exhibit is a verbatim copy of an input or output file provided to assist in understanding how the input file is prepared for a specific problem and to show complete file examples. Line numbers are provided on the left side of each exhibit; these are not a part of the actual file. The line numbers are available only to aid in reading the input file and referencing portions of it in the discussion. When the line that appears in an input file is too wide to display in this document, the continuation is shown indented on the subsequent line without a line number.

Where comparisons are made to analytical or semi-analytical results, the relative root mean square (*RRMS*) was adopted as the performance indicator. This statistic is computed as

$$RRMS = \sqrt{\frac{\sum_{i=1}^{k}\left(\frac{\alpha_i - n_i}{\alpha_i}\right)^2}{k}} \tag{8.1}$$

where α_i = analytic solution parameter value (e.g., liquid saturation) at point i, n_i = numerical solution parameter value (liquid saturation) at point i, and k = number of comparison points. To judge the accuracy level of this verification test, the performance categories set by Baca and Magnuson (1990) are adopted. These ranges are "somewhat arbitrary but nevertheless represent a consistent basis for evaluating the quality of the comparison" (Baca and Magnuson 1990). The ranges are:

- Excellent - *RRMS* ≤ 0.01
- Good- *RRMS* ≤ 0.05
- Acceptable- *RRMS* ≤ 0.10
- Unacceptable- *RRMS* > 0.10

Table 8.1. Summary of Sample Problems

	Problem Description	Dimensions	Solution Mode	Issues
1	Single-Node Evaporation	1	Energy	phase transitions, component appearance and disappearance, mass conservation
2	Single-Node Condensation	1	Energy	phase transitions, component appearance and disappearance, mass conservation
3	Hot Two-Phase Flow	1	Water-Air-Energy	energy conservation
4	Philip's Vertical Infiltration	1	Water	code verification against semi-analytic solution (Philip 1957)
5	Two-Dimensional Infiltration	2	Water	code comparison to numerical results (Pruess 1987)
6	Two-Phase Infiltration	1	Water, Water-Air	air-flow effects on water infiltration; code comparison to experimental and numerical results (Touma and Vauclin 1986)
7	One-Dimensional Heat Pipe	1	Water-Air-Energy	code verification against known semi-analytical solution (Udell and Fitch 1985)
8	Unsaturated Transport	1	Water (Species)	code verification against semi-analytical solution (Ross et al. 1982; Smiles et al. 1977)

8.1 Single-Node Evaporation

The single-node-evaporation problem involves the evaporation of liquid water within a closed adiabatic volume of partially saturated porous medium. The evaporation process occurs through the addition of heat into the control volume. Sufficient heat is added to the system to desaturate the porous medium. Because the control volume surfaces are closed and adiabatic, the initial quantities of air and water mass should remain constant throughout the simulation. Upon desaturation of a node, MSTS switches the primary variable for the water mass conservation equation from the liquid pressure to the water-vapor mass fraction. This problem demonstrates this numerical transition from two-phase conditions to gas-phase-only conditions. The problem requires the coupled solution of the water mass, air mass, and energy conservation equations.

8.1.1 Problem Domain and Input Parameters

This problem involves a 10-m^3 cube of porous media, with a total porosity of 0.50, rock density of 2650 kg/m^3, and specific heat of 1000 J/kg K. The initial gas pressure, liquid saturation, and temperature are 10^5 Pa (absolute), 0.01, and 90°C, respectively. A constant internal heat source of 2 MW was applied. All boundary surfaces are adiabatic, no-flow surfaces. A complete description of the problem specifics is given in the "input" file shown in Exhibit 8.1.

8.1.2 Simulation Results

Simulation results in terms of the system temperature and liquid saturation are shown in Figure 8.1. The system begins at an initially fully saturated state, and liquid saturation declines with time to a completely desaturated state as water undergoes phase change with increasing temperature. The simulation is halted at 1875 seconds at a final temperature of 363.9°C, which is slightly below the critical temperature for water. The output file generated by MSTS for the single-node-evaporation problem is shown in Exhibit 8.2.

8.1.3 Mass Balance Check

This problem concerns a closed system in which mass must be conserved. To test that MSTS conserves mass in simulating a phase change, a mass balance check was performed. The check compares the total mass of water in the cube represented by the single node at the initial conditions to the total mass of water at 1875 seconds, the end of the simulation time. The total mass of water in the node (m_T^w) is the sum of the water in the aqueous (m_ℓ^w) and vapor (m_g^w) phases.

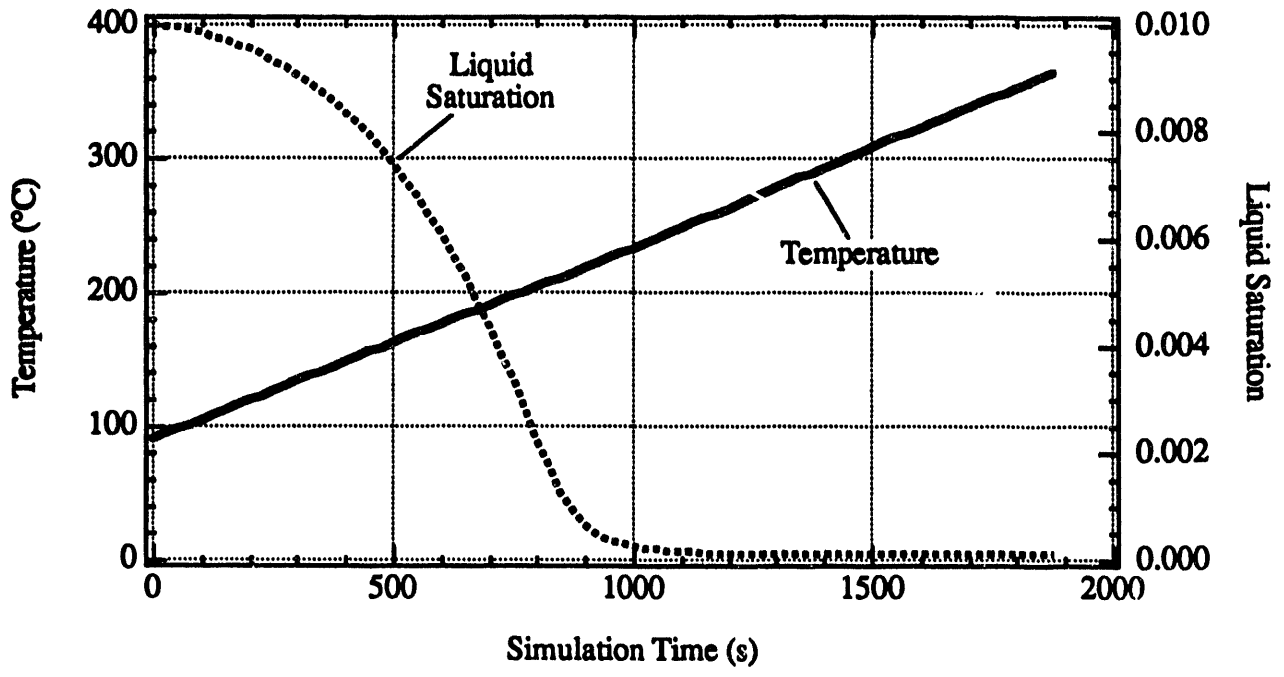

Figure 8.1. MSTS-Predicted Temperature and Liquid Saturation Variation with Time for the Single-Node-Evaporation Problem

The mass of water in the aqueous phase is given by

$$m_\ell^w = \eta_D V \rho_\ell = (n_T - n_D + s_\ell n_D) V \rho_\ell \tag{8.2}$$

and the mass of water in the gas phase by

$$m_g^w = (1 - s_\ell) n_D V x_\ell^w \rho_g \tag{8.3}$$

In mathematical terms, the total mass in the domain is the sum of the water in each phase:

$$m_T^w = m_\ell^w + m_g^w \tag{8.4}$$

The initial conditions were derived from the problem definition and the final conditions were obtained from the plot file generated by the MSTS code; both are shown in Table 8.2. Substituting the values from Table 8.2 into Equation (8.2), the total water mass in the aqueous phase at time zero (initial) is

$$\begin{aligned} m_\ell^w &= (n_T - n_D + s_\ell n_D) V \rho_\ell \\ &= [0.50 - 0.50 + (0.01)(0.50)] (10\ \text{m}^3)(965.1\ \text{kg/m}^3) \\ &= 48.255\ \text{kg} \end{aligned}$$

Table 8.2. Single-Node-Evaporation Problem Initial and Final Conditions

Variable	Units	Initial Conditions	Final Conditions
V	m^3	10.0	10.0
n_T	-	0.50	0.50
n_D	-	0.50	0.50
T	°C	90.0	363.86
s_ℓ	-	0.01	9.6219×10^{-5}
ρ_ℓ	kg/m^3	965.1	473.72
ρ_g	kg/m^3	0.7102	10.307
x_ℓ^w	-	0.5964	0.97170

Substituting values from Table 8.2 into Equation (8.3), the water mass in the gas phase at time zero is

$$\begin{aligned} m_g^w &= (1 - s_\ell)\, n_D V\, x_g^w\, \rho_g \\ &= (1 - 0.01)\,(0.50)\,(10\ m^3)\,(0.5964)\,(0.7102\ kg/m^3) \\ &= 2.09664\ kg \end{aligned}$$

Therefore, the total water mass in the node at time zero is 50.352 kg. When the simulation is completed, the temperature is 363.9°C and the water mass in the aqueous phase is

$$\begin{aligned} m_\ell^w &= (n_T - n_D + s_\ell n_D)\, V\, \rho_\ell \\ &= \left[0.50 - 0.50 + \left(9.6219 \times 10^{-5}\right)(0.50)\right](10\ m^3)\,(473.72\ kg/m^3) \\ &= 0.2279\ kg \end{aligned}$$

(i.e., there is essentially no water mass in the aqueous phase) and the water mass in the gas phase is

$$\begin{aligned} m_g^w &= (1 - s_\ell)\, n_D V\, x_g^w\, \rho_g \\ &= \left(1 - 9.6219 \times 10^{-5}\right)(0.50)\,(10\ m^3)\,(0.97170)\,(10.307\ kg/m^3) \\ &= 50.0717\ kg \end{aligned}$$

These two values sum to a total water mass in the node at final conditions of 50.300 kg. The mass difference between initial and final conditions is therefore 50.352 - 50.300 = 0.052 kg, or 0.10%.

Exhibit 8.1. MSTS Input File for Single-Node-Evaporation Problem

Line No.	Input File
1	~Simulation Title and Notes
2	beta,0001,
3	Single-Node-Evaporation Problem
4	L.E. Peele
5	Battelle, Pacific Northwest Laboratory
6	Wednesday, July 1, 1992
7	2:43:50 PM
8	32 character(s) of simulation title notes follows.
9	Single-node-evaporation problem.
10	~Solution Schemes
11	false,false,false,
12	banded matrix
13	true,true,true,false,
14	1875.,s,
15	25.0,s,
16	1.0,
17	25.0,s,
18	true,true,false,true,true,true,
19	false,false,false,false,
20	~Numerical Control
21	8,Maximum Residual,
22	1.0,h,1.0,h,
23	1.0e-6,1.0e-6,1.0e-6,
24	Harmonic Mean,Harmonic Mean,Harmonic Mean,Harmonic Mean,
25	~Grid Geometry
26	cartesian
27	1,1,1,
28	2.1544,m,2.1544,m,2.1544,m,0.0,m,0.0,m,
29	0.0,m,
30	1 line(s) of grid geometry input follows.
31	Node 1,1.0772,m,
32	1 line(s) of grid geometry input follows.
33	Node 1,1.0772,m,
34	1 line(s) of grid geometry input follows.
35	Node 1,1.0772,m,
36	~Inactive Nodes
37	0 line(s) of inactive nodes input follows.
38	~Rock or Soil Types
39	0 character(s) of rock or soil types notes follows.
40	1 line(s) of rock or soil types input follows.
41	Generic Sand,1,1,1,1,1,1,
42	~Mechanical Properties
43	1 line(s) of mechanical properties input follows.
44	Generic Sand,0.5,0.5,0.5,,,,dependent,,,
45	~Hydraulic Properties
46	1 line(s) of hydraulic properties input follows.
47	Generic Sand,1.0E-14,1.0E-14,1.0E-14,m^2,,,,m^2,0.0,1/m,
48	~Thermal Properties
49	1 line(s) of thermal properties input follows.
50	Generic Sand,dependent,2.10,2.10,2.10,,,,W/m K,2650.0,kg/m^3,1000.0,J/kg K,
51	~Species Properties
52	0 line(s) of species properties input follows.
53	~Soil Characteristics
54	1 line(s) of soil characteristics input follows.
55	Generic Sand,van Genuchten,0.5,1/m,2.0,1.0E+6,m,,,,
56	~Liquid Relative Permeability Properties
57	1 line(s) of liquid relative permeability input follows.
58	Generic Sand,Corey's Curves,0.30,0.05,1.0E-10,,
59	~Gas Relative Permeability Properties
60	0 line(s) of gas relative permeability input follows.
61	~Liquid Boundary Conditions
62	0 line(s) of liquid boundary conditions input follows.
63	~Gas Boundary Conditions

Exhibit 8.1. (Contd)

Line No.	Input File
64	0 line(s) of gas boundary conditions input follows.
65	~Vapor Boundary Conditions
66	0 line(s) of vapor boundary conditions input follows.
67	~Energy Boundary Conditions
68	0 line(s) of energy boundary conditions input follows.
69	~Species Boundary Conditions
70	0 line(s) of species boundary conditions input follows.
71	~Initial Conditions
72	Liquid Saturation & Gas Pressure,
73	3 line(s) of initial conditions input follows.
74	Gas Pressure,1.0E+5,Pa (absolute),,1/m,,1/m,,1/m,1,1,1,1,1,1,
75	Liquid Saturation,0.01,,,1/m,,1/m,,1/m,1,1,1,1,1,1,
76	Temperature,90.0,Celsius,,1/m,,1/m,,1/m,1,1,1,1,1,1,
77	~Sources & Sinks
78	1 line(s) of sources & sinks input follows.
79	Thermal Energy,Constant,2.0E+5,W/m^3,,,,,0,s,1875.0,s,1,1,1,1,1,1,
80	~Liquid Pathline Trace
81	0 line(s) of liquid pathline trace input follows.
82	~Output Control
83	1,1,1,1,1,1,zxplane,
84	0 line(s) of output control input follows.
85	1,1,1,,,,,,,,,,1,
86	3 line(s) of output control input follows.
87	Liquid Pressure,
88	Temperature,
89	Liquid Saturation,
90	8 line(s) of output control input follows.
91	Liquid Pressure,
92	Gas Pressure,
93	Temperature,
94	Liquid Saturation,
95	Liquid Phase Air Mass Fraction,
96	Gas Phase Vapor Mass Fraction,
97	Liquid Density,
98	Gas Density,
99	3 line(s) of output control input follows.
100	Liquid Pressure,
101	Temperature,
102	Liquid Saturation,
103	~Surface Flux Integrator
104	0 line(s) of surface flux integrator input follows.
105	~Rock List
106	1 line(s) of rock list input follows.
107	Generic Sand,
108	~

Exhibit 8.2. MSTS Output File for Single-Node-Evaporation Problem

Line No. **Output File**

```
 1
 2
 3
 4                MM       MM   SSSSS S  TTTTTTTTT   SSSSS S
 5                 MM     MM   S     SS  T   T   T  S     SS
 6                 M M   M M   SS     S      T      SS     S
 7                 M  M M  M     SSSS        T        SSSS
 8                 M   M   M   S     SS      T      S     SS
 9                 M       M   SS     S      T      SS     S
10                MMM     MMM  S SSSSS      TTT     S SSSSS
11
12
13
14    ******************************************************************************
15
16            THIS OUTPUT FILE WAS PRODUCED BY THE NUMERICAL MODEL
17
18            --------------------- M S T S ----------------------
19
20                MULTIPHASE SUBSURFACE TRANSPORT SIMULATOR
21
22            ---------------------------------------------------
23
24            DEVELOPED BY BATTELLE, PACIFIC NORTHWEST LABORATORY
25
26            ---------------------------------------------------
27
28            THIS COMPUTER CODE WAS DEVELOPED UNDER CONTRACT TO
29
30                  THE UNITED STATES DEPARTMENT OF ENERGY
31
32            ---------------------------------------------------
33
34            FOR ENQUIRIES OR ASSISTANCE: CALL 509 375-2183 USA
35                                           OR  509 376-8315 USA
36
37                VERSION: beta    REVISION: 0001
38
39                EXECUTION DATE: 12/ 7/1992
40
41                EXECUTION TIME: 15:45: 5
42
43                EXECUTION IDENTIFICATION: 12 7921545
44
45            RESULTS FROM THIS VERSION OF MSTS SHOULD NOT BE USED
46            FOR LICENSE RELATED APPLICATIONS.
47
48    ******************************************************************************
49
50
51
52    RECORD OF INPUT DATA
53    --------------------
54
55
56    Simulation Title and Notes
57    --------------------------
58    Simulation Title:    Single-Node-Evaporation Problem
59    User Name:           L.E. Peele
60    Company Name:        Battelle, Pacific Northwest Laboratory
61    Input Creation Date: Wednesday, July 1, 1992
62    Input Creation Time: 2:43:50 PM
63
```

Line No. Output File

```
 64
 65     Simulation notes:
 66
 67
 68    Single-node-evaporation problem.
 69
 70
 71     Solution Schemes and Options
 72     ----------------------------
 73     Solution Algorithm: Banded Matrix
 74     Simulation Control: Full Execution
 75     Simulation Type:    New Simulation
 76
 77
 78    Solved Equations:
 79     Thermal Energy Equation: solution on
 80     Water Equation:          solution on
 81     Air Equation:            solution on
 82     Species Conc. Equation:   solution off
 83
 84
 85    Time Advancement and Limits
 86     Maximum Time:                    1.8750E+03
 87     Initial Time Step:               2.5000E+01
 88     Time Step Acceleration Factor:   1.0000E+00
 89     Maximum Time Step:               2.5000E+01
 90
 91
 92    Solution Options
 93     Screen Printing:           On
 94     Binary Diffusion:          On
 95     Fixed Physical Properties: Off
 96     Liquid Phase:              On
 97     Gas Phase:                 On
 98     Vapor Pressure Lowering:   On
 99
100
101     Numerical Control
102     -----------------
103
104
105    Convergence criteria
106     Maximum Number of Iterations per Step :    8
107     Convergence Mode Index: Maximum Residual
108     CPU Limit, s:    3.6000E+03
109     Clock Limit, s:  3.6000E+03
110     Temperature Residual:                    1.0000E-06
111     Liquid Pressure Residual:                1.0000E-06
112     Gas Pressure Residual:                   1.0000E-06
113
114
115    Node Boundary Averaging Schemes
116     Thermal Energy Equation:        harmonic mean
117     Liquid Phase:                   harmonic mean
118     Gas Phase:                      harmonic mean
119     Species Concentration Equation: harmonic mean
120
121
122     Grid Geometry
123     -------------
124    Grid Type: Cartesian
125
126
```

Exhibit 8.2. (Contd)

Line No.	Output File

```
127   Grid Dimensions
128    Number of X-direction Nodes:        1
129    Number of Y-direction Nodes:        1
130    Number of Z-direction Nodes:        1
131
132
133   Physical Dimensions
134    X-direction Length,m:          2.1544E+00
135    Y-direction Length,m:          2.1544E+00
136    Z-direction Length,m:          2.1544E+00
137    Z-direction Datum,m:           0.0000E+00
138    Grid Bottom Elevation,m:       0.0000E+00
139      Inner Radius Length, m: 0.0000E+00
140
141
142   X-Direction Node Positions
143    Node:    1 Node Position, m:  1.0772E+00
144
145
146   Y-Direction Node Positions
147    Node:    1 Node Position, m:  1.0772E+00
148
149
150   Z-Direction Node Positions
151    Node:    1 Node Position, m:  1.0772E+00
152
153
154    Rock or Soil Types
155    ------------------
156    Rock Notes:
157
158
159
160
161    Rock Types and Domains
162      Rock Number:      1
163      Rock Type: generic sand
164      Rock Domain: I =      1 to      1
165                   J =      1 to      1
166                   K =      1 to      1
167
168
169    Mechanical Properties
170    ---------------------
171
172
173    Rock type: generic sand
174    Total Porosity:                5.0000E-01
175    Diffusive Porosity:            5.0000E-01
176    Effective Porosity:            5.0000E-01
177    Saturation Dependent Tortuosities
178    Liquid Phase Tortuosity: Millington and Quirk Model
179    Gas Phase Tortuosity:    Millington and Quirk Model
180
181
182    Hydraulic Properties
183    --------------------
184
185
186    Rock type:generic sand
187    X-Direction Intrinsic Permeability, m^2: 1.0000E-14
188    Y-Direction Intrinsic Permeability, m^2: 1.0000E-14
189    Z-Direction Intrinsic Permeability, m^2: 1.0000E-14
```

Exhibit 8.2. (Contd)

Line No.	Output File
190	Specific Storativity, 1/m: 0.0000E+00
191	Porous Media Compressibility, 1/Pa: 0.0000E+00
192	
193	
194	Thermal Properties
195	----------
196	
197	
198	Rock type: generic sand
199	Rock Thermal Conductivity Model: Temperature Dependent
200	X-Dir. Unsaturated Thermal Cond., W/m K: 2.1000E+00
201	Y-Dir. Unsaturated Thermal Cond., W/m K: 2.1000E+00
202	Z-Dir. Unsaturated Thermal Cond., W/m K: 2.1000E+00
203	Rock Density, kg/m^3: 2.6500E+03
204	Specific heat, J/kg K: 1.0000E+03
205	
206	
207	Species Properties
208	----------
209	
210	
211	Soil Characteristics
212	----------
213	
214	
215	Rock type: generic sand
216	Characteristic Function: van Genuchten
217	van Genuchten [Alpha] Parameter, 1/m: 5.0000E-01
218	van Genuchten [Beta] Parameter: 2.0000E+00
219	Maximum Tension Head, m: 1.0000E+06
220	
221	
222	Liquid Relative Permeability
223	----------
224	
225	
226	Rock type: generic sand
227	Liquid Relative Permeability Function: Corey's Curves
228	Residual Saturation: 3.0000E-01
229	Entrapped Air Saturation: 5.0000E-02
230	Minimum Liquid Relative Permeability: 1.0000E-10
231	
232	
233	Gas Relative Permeability Functions
234	----------
235	
236	
237	Liquid Boundary Conditions
238	----------
239	
240	
241	Gas Boundary Conditions
242	----------
243	
244	
245	Vapor Boundary Conditions
246	----------
247	
248	
249	Thermal Energy Boundary Conditions
250	----------
251	
252	

Exhibit 8.2. (Contd)

Line No.	Output File
253	Species Boundary Conditions
254	----------
255	
256	
257	Initial Conditions
258	----------
259	Initial Saturation Option: liquid saturation & gas pressure
260	
261	
262	Gas Pressure (absolute), Pa
263	PG(1, 1, 1): 1.0000E+05
264	X-direction Gradient: 0.0000E+00
265	Y-direction Gradient: 0.0000E+00
266	Z-direction Gradient: 0.0000E+00
267	Domain: I = 1 to 1
268	J = 1 to 1
269	K = 1 to 1
270	
271	
272	Liquid Saturation
273	SL(1, 1, 1): 1.0000E-02
274	X-direction Gradient: 0.0000E+00
275	Y-direction Gradient: 0.0000E+00
276	Z-direction Gradient: 0.0000E+00
277	Domain: I = 1 to 1
278	J = 1 to 1
279	K = 1 to 1
280	
281	
282	Temperature, C
283	T(1, 1, 1): 9.0000E+01
284	X-direction Gradient: 0.0000E+00
285	Y-direction Gradient: 0.0000E+00
286	Z-direction Gradient: 0.0000E+00
287	Domain: I = 1 to 1
288	J = 1 to 1
289	K = 1 to 1
290	
291	
292	Sources and Sinks
293	----------
294	Thermal Energy Source
295	Temporal Variation: Constant
296	Source Power Density, W/m^3: 2.0000E+05
297	Source Start Time, s: 0.0000E+00
298	Source Stop Time, s: 1.8750E+03
299	Domain: I = 1 to 1
300	J = 1 to 1
301	K = 1 to 1
302	
303	
304	Output Control
305	----------
306	
307	
308	Output File Variables
309	
310	
311	liquid pressure
312	temperature
313	liquid saturation
314	
315	

Exhibit 8.2. (Contd)

Line No. Output File

```
316   Plot File Variables
317
318
319     liquid pressure
320     gas pressure
321     temperature
322     liquid saturation
323     liquid phase air mass fraction
324     gas phase vapor mass fraction
325     liquid density
326     gas density
327
328
329   Reference Node File Variables
330
331
332     liquid pressure
333     temperature
334     liquid saturation
335
336
337    Field Variable Output Frequency:
338       After the Final Time Step
339
340
341    Output Orientation: Z-X Planes
342    Output Domain: I =    1 to    1
343                   J =    1 to    1
344                   K =    1 to    1
345
346
347    Reference Node No.     1: I =      1, J =      1, K =      1
348    Reference Node Output Frequency: Every      1 Time Step(s)
349
350
351
352    REFERENCE NODE OUTPUT RECORD
353    ----------------------------
354
355    REFERENCE NODE(S) (  1,  1,  1)
356
357     STEP   TIME     ITER  EQUA   TIMESTEP       P           T           SL
358       0  0.000E+00   0     0    2.500E+01  -1.859E+06  9.000E+01  1.000E-02
359       1  2.500E+01   3     3    2.500E+01  -1.855E+06  9.367E+01  9.967E-03
360       2  5.000E+01   3     3    2.500E+01  -1.851E+06  9.734E+01  9.928E-03
361       3  7.500E+01   3     2    2.500E+01  -1.847E+06  1.010E+02  9.882E-03
362       4  1.000E+02   3     2    2.500E+01  -1.843E+06  1.047E+02  9.829E-03
363       5  1.250E+02   3     2    2.500E+01  -1.839E+06  1.083E+02  9.768E-03
364       6  1.500E+02   3     2    2.500E+01  -1.836E+06  1.120E+02  9.698E-03
365       7  1.750E+02   3     2    2.500E+01  -1.833E+06  1.156E+02  9.620E-03
366       8  2.000E+02   3     2    2.500E+01  -1.830E+06  1.192E+02  9.531E-03
367       9  2.250E+02   3     2    2.500E+01  -1.828E+06  1.229E+02  9.432E-03
368      10  2.500E+02   3     2    2.500E+01  -1.827E+06  1.265E+02  9.321E-03
369      11  2.750E+02   3     2    2.500E+01  -1.827E+06  1.301E+02  9.199E-03
370      12  3.000E+02   3     2    2.500E+01  -1.829E+06  1.337E+02  9.063E-03
371      13  3.250E+02   4     3    2.500E+01  -1.832E+06  1.373E+02  8.914E-03
372      14  3.500E+02   4     3    2.500E+01  -1.837E+06  1.409E+02  8.749E-03
373      15  3.750E+02   4     3    2.500E+01  -1.846E+06  1.445E+02  8.570E-03
374      16  4.000E+02   4     2    2.500E+01  -1.858E+06  1.480E+02  8.373E-03
375      17  4.250E+02   4     2    2.500E+01  -1.874E+06  1.516E+02  8.159E-03
376      18  4.500E+02   4     2    2.500E+01  -1.896E+06  1.552E+02  7.927E-03
377      19  4.750E+02   4     2    2.500E+01  -1.925E+06  1.587E+02  7.675E-03
378      20  5.000E+02   4     2    2.500E+01  -1.964E+06  1.622E+02  7.402E-03
```

Exhibit 8.2. (Contd)

Line No. Output File

```
379      21  5.250E+02   4     2     2.500E+01  -2.014E+06  1.658E+02  7.108E-03
380      22  5.500E+02   4     2     2.500E+01  -2.080E+06  1.693E+02  6.791E-03
381      23  5.750E+02   4     2     2.500E+01  -2.165E+06  1.728E+02  6.450E-03
382
383    REFERENCE NODE(S) (  1,  1,  1)
384
385     STEP    TIME     ITER  EQUA   TIMESTEP        P          T          SL
386      24  6.000E+02   4     2     2.500E+01  -2.275E+06  1.763E+02  6.085E-03
387      25  6.250E+02   4     2     2.500E+01  -2.420E+06  1.798E+02  5.695E-03
388      26  6.500E+02   4     2     2.500E+01  -2.612E+06  1.832E+02  5.278E-03
389      27  6.750E+02   4     2     2.500E+01  -2.868E+06  1.867E+02  4.834E-03
390      28  7.000E+02   4     2     2.500E+01  -3.217E+06  1.901E+02  4.363E-03
391      29  7.250E+02   4     2     2.500E+01  -3.700E+06  1.936E+02  3.867E-03
392      30  7.500E+02   4     2     2.500E+01  -4.391E+06  1.970E+02  3.347E-03
393      31  7.750E+02   4     2     2.500E+01  -5.415E+06  2.005E+02  2.808E-03
394      32  8.000E+02   5     2     2.500E+01  -6.997E+06  2.039E+02  2.262E-03
395      33  8.250E+02   5     2     2.500E+01  -9.550E+06  2.074E+02  1.732E-03
396      34  8.500E+02   5     2     2.500E+01  -1.375E+07  2.109E+02  1.256E-03
397      35  8.750E+02   5     2     2.500E+01  -2.031E+07  2.144E+02  8.807E-04
398      36  9.000E+02   4     2     2.500E+01  -2.938E+07  2.180E+02  6.245E-04
399      37  9.250E+02   4     2     2.500E+01  -4.032E+07  2.217E+02  4.625E-04
400      38  9.500E+02   4     2     2.500E+01  -5.239E+07  2.254E+02  3.596E-04
401      39  9.750E+02   4     2     2.500E+01  -6.512E+07  2.291E+02  2.914E-04
402      40  1.000E+03   4     2     2.500E+01  -7.824E+07  2.328E+02  2.437E-04
403      41  1.025E+03   3     2     2.500E+01  -9.158E+07  2.365E+02  2.090E-04
404      42  1.050E+03   3     2     2.500E+01  -1.051E+08  2.402E+02  1.826E-04
405      43  1.075E+03   3     2     2.500E+01  -1.187E+08  2.440E+02  1.620E-04
406      44  1.100E+03   3     2     2.500E+01  -1.323E+08  2.477E+02  1.455E-04
407      45  1.125E+03   3     2     2.500E+01  -1.461E+08  2.515E+02  1.321E-04
408      46  1.150E+03   3     2     2.500E+01  -1.598E+08  2.552E+02  1.208E-04
409      47  1.175E+03   3     2     2.500E+01  -1.736E+08  2.589E+02  1.114E-04
410
411    REFERENCE NODE(S) (  1,  1,  1)
412
413     STEP    TIME     ITER  EQUA   TIMESTEP        P          T          SL
414      48  1.200E+03   3     2     2.500E+01  -1.874E+08  2.627E+02  1.032E-04
415      49  1.225E+03   3     2     2.500E+01  -2.012E+08  2.664E+02  9.622E-05
416      50  1.250E+03   3     3     2.500E+01  -2.012E+08  2.702E+02  9.622E-05
417      51  1.275E+03   3     3     2.500E+01  -2.012E+08  2.739E+02  9.622E-05
418      52  1.300E+03   3     3     2.500E+01  -2.012E+08  2.777E+02  9.622E-05
419      53  1.325E+03   3     3     2.500E+01  -2.011E+08  2.814E+02  9.622E-05
420      54  1.350E+03   3     3     2.500E+01  -2.011E+08  2.852E+02  9.622E-05
421      55  1.375E+03   3     3     2.500E+01  -2.011E+08  2.889E+02  9.622E-05
422      56  1.400E+03   3     3     2.500E+01  -2.011E+08  2.927E+02  9.622E-05
423      57  1.425E+03   3     3     2.500E+01  -2.011E+08  2.964E+02  9.622E-05
424      58  1.450E+03   3     3     2.500E+01  -2.010E+08  3.002E+02  9.622E-05
425      59  1.475E+03   3     3     2.500E+01  -2.010E+08  3.039E+02  9.622E-05
426      60  1.500E+03   3     3     2.500E+01  -2.010E+08  3.076E+02  9.622E-05
427      61  1.525E+03   3     3     2.500E+01  -2.010E+08  3.114E+02  9.622E-05
428      62  1.550E+03   3     3     2.500E+01  -2.010E+08  3.151E+02  9.622E-05
429      63  1.575E+03   3     2     2.500E+01  -2.009E+08  3.189E+02  9.622E-05
430      64  1.600E+03   3     3     2.500E+01  -2.009E+08  3.226E+02  9.622E-05
431      65  1.625E+03   3     3     2.500E+01  -2.009E+08  3.264E+02  9.622E-05
432      66  1.650E+03   3     3     2.500E+01  -2.009E+08  3.301E+02  9.622E-05
433      67  1.675E+03   3     3     2.500E+01  -2.009E+08  3.339E+02  9.622E-05
434      68  1.700E+03   3     3     2.500E+01  -2.008E+08  3.376E+02  9.622E-05
435      69  1.725E+03   3     3     2.500E+01  -2.008E+08  3.414E+02  9.622E-05
436      70  1.750E+03   3     3     2.500E+01  -2.008E+08  3.451E+02  9.622E-05
437      71  1.775E+03   3     3     2.500E+01  -2.008E+08  3.489E+02  9.622E-05
438
439    REFERENCE NODE(S) (  1,  1,  1)
440
441     STEP    TIME     ITER  EQUA   TIMESTEP        P          T          SL
```

Exhibit 8.2. (Contd)

Line No. Output File

```
442      72  1.800E+03   3     3    2.500E+01  -2.008E+08  3.526E+02  9.622E-05
443      73  1.825E+03   3     3    2.500E+01  -2.007E+08  3.564E+02  9.622E-05
444      74  1.850E+03   3     3    2.500E+01  -2.007E+08  3.601E+02  9.622E-05
445      75  1.875E+03   3     3    2.500E+01  -2.007E+08  3.639E+02  9.622E-05
446
447
448   FIELD AND FLUX VARIABLE RESULTS @
449   --------------------------------
450            75 steps
451    1.8750E+03 s
452    5.2083E-01 h
453    2.1701E-02 day
454    3.1002E-03 wk
455    5.9415E-05 yr
456
457   Execution time from start:  0: 0:12
458   Execution performance, s/node/step : 1.6173E-01
459
460
461   1
462   0        Liquid Pressure (absolute), Pa
463   0           j =    1
464        Distance =   1.077 m
465
466           Node   Dist.      1.077 m
467            No.    m           =   1
468
469        i =    1    1.077  -2.0071E+08
470   0
471   1
472   0        Temperature, C.
473   0           j =    1
474        Distance =   1.077 m
475
476           Node   Dist.      1.077 m
477            No.    m           =   1
478
479        i =    1    1.077   3.6386E+02
480   0
481   1
482   0        Liquid Saturation.
483   0           j =    1
484        Distance =   1.077 m
485
486           Node   Dist.      1.077 m
487            No.    m           =   1
488
489        i =    1    1.077   9.6219E-05
490   0
491
492    END OF SIMULATION
493    -----------------
```

8.2 Single-Node Condensation

The single-node-condensation problem involves the condensation of water vapor within a closed adiabatic volume of porous medium initially desaturated. The condensation process occurs through the removal of heat from the control volume. Sufficient heat is removed from the system to cause condensation and partially saturate the porous medium. Because the control volume surfaces are closed and adiabatic, the initial quantities of air and water mass should remain constant throughout the simulation. Upon partial saturation of a desaturated node, MSTS switches the primary variable for the water mass conservation equation from the the water-vapor mass fraction to the liquid pressure. This problem demonstrates this numerical transition from gas-phase-only conditions to two-phase conditions. The problem requires the coupled solution of the water mass, air mass, and energy conservation equations.

8.2.1 Problem Domain and Input Parameters

This problem involves a 10-m^3 cube of porous media, with a total porosity of 0.50, rock density of 2650 kg/m^3, and specific heat of 1000 J/kg K. The initial gas pressure, liquid saturation, and temperature are 4 MPa (absolute), 2×10^{-8}, and 280°C, respectively. A constant internal heat removal rate of -0.5 MW was applied. All boundary surfaces are adiabatic, no-flow surfaces. A complete description of the problem specifics is given in the "input" file shown in Exhibit 8.3.

8.2.2 Simulation Results

Simulation results in terms of the system temperature and liquid saturation are shown in Figure 8.2. The liquid saturation remains at zero (the initial condition) until near 1000 seconds, at which time the numerical switch of primary variables occurs when temperature has declined to a point where phase change from gas to aqueous begins. The simulation is halted at 1875 seconds at a final temperature of 214.7°C.

8.2.3 Mass Balance Check

As for the single-node-evaporation problem, this problem concerns a closed system in which mass must be conserved. The mass balance check is repeated for the condensation problem using Equations (8.2) through (8.4) with values from the single-node-condensation problem (Table 8.3). For the initial conditions, the mass of water in the aqueous phase is computed as

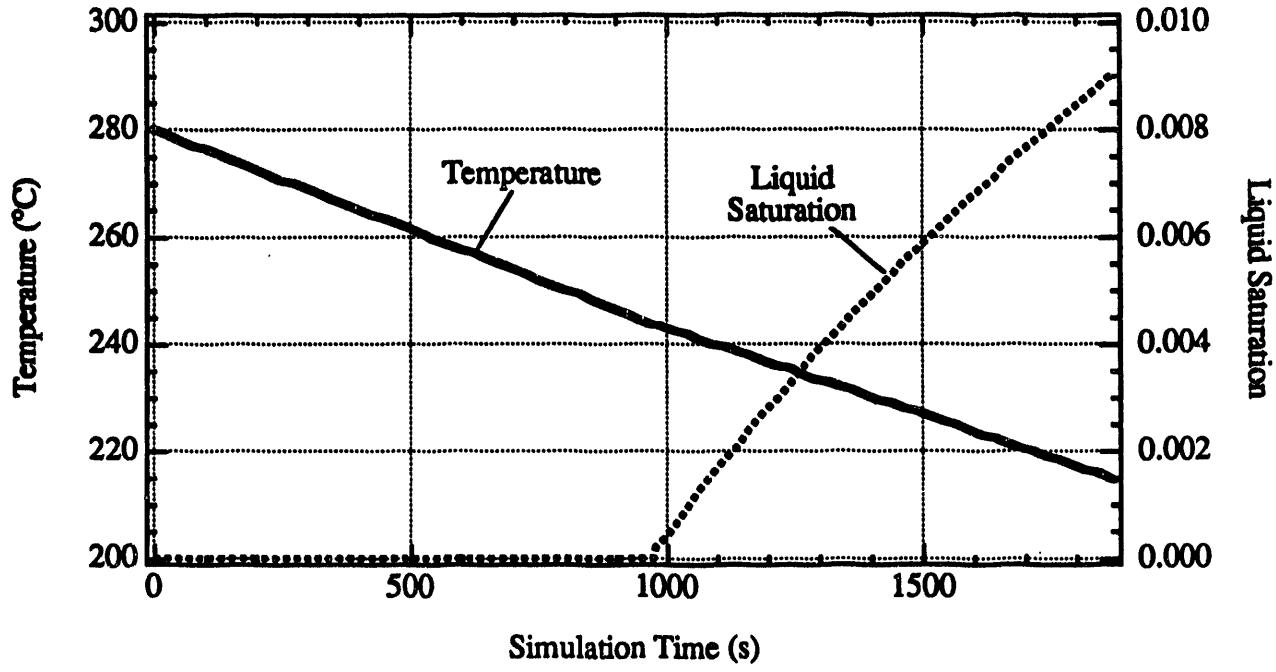

Figure 8.2. MSTS-Predicted Temperature and Liquid Saturation Variation with Time for the Single-Node-Condensation Problem

Table 8.3. Single-Node-Condensation Problem Initial and Final Conditions

Variable	Units	Initial Conditions	Final Conditions
V	m^3	10.0	10.0
n_T	-	0.50	0.50
n_D	-	0.50	0.50
T	°C	280.00	214.68
s_ℓ	-	0.000000	0.009000
ρ_ℓ	kg/m^3	746.3	847.1
ρ_g	kg/m^3	18.04	10.64
x_ℓ^w	-	1.0000	1.0000

$$m_\ell^w = (n_T - n_D + s_\ell n_D)\, V\, \rho_\ell$$
$$= [0.50 - 0.50 + (0.0)\,(0.50)]\,(10\ \mathrm{m}^3)\,(746.3\ \mathrm{kg/m}^3)$$
$$= 0.0\ \mathrm{kg}$$

(i.e., there is no water in the aqueous phase), while the water mass in the gas phase at time zero is

$$m_g^w = (1 - s_\ell)\, n_D\, V\, x_\ell^w\, \rho_g$$
$$= (1 - 0.0)\,(0.50)\,(10\ \mathrm{m}^3)\,(1.0)\,(18.04\ \mathrm{kg/m}^3)$$
$$= 90.200\ \mathrm{kg}$$

Therefore, the total water mass at the start of the simulation period is 90.200 kg. At the end of the simulation (after 1875 seconds), the temperature is reduced to 214.7 °C and the water mass in the aqueous phase is

$$m_\ell^w = (n_T - n_D + s_\ell n_D)\, V\, \rho_\ell$$
$$= [0.50 - 0.50 + (0.0090)\,(0.50)]\,(10\ \mathrm{m}^3)\,(847.1\ \mathrm{kg/m}^3)$$
$$= 38.120\ \mathrm{kg}$$

while the water mass remaining in the gas phase is

$$m_g^w = (1 - s_\ell)\, n_D\, V\, x_\ell^w\, \rho_g$$
$$= (1 - 0.0090)\,(0.50)\,(10\ \mathrm{m}^3)\,(1.0)\,(10.64\ \mathrm{kg/m}^3)$$
$$= 52.721\ \mathrm{kg}$$

Summing, the total water mass in the system at the end of the simulation is 38.120 + 52.721 = 90.841 kg. The difference between initial and final mass is 90.200 - 90.841 = -0.641 kg, which is 0.71% of the initial mass.

Exhibit 8.3. MSTS Input File for Single-Node-Condensation Problem

Line No.	Input File
1	~Simulation Title and Notes
2	beta,0001,
3	Single-Node-Condensation Problem
4	L.E. Peele
5	Battelle, Pacific Northwest Laboratory
6	Wednesday, June 24, 1992
7	1:19:00 PM
8	245 character(s) of simulation title notes follows.
9	Single-node-condensation problem. A vapor-pressure-lowering scheme will be used
10	to restrict the minimum liquid saturation level. This problem will test the ab
11	ility of the Newton-Raphson scheme to handle low air mass fractions in the gas p
12	hase.
13	~Solution Schemes
14	false,false,false,
15	banded matrix
16	true,true,true,false,
17	1875.,s,
18	25.0,s,
19	1.5,
20	25.0,s,
21	true,true,false,true,true,false,
22	false,false,false,false,
23	~Numerical Control
24	8,Maximum Residual,
25	1.0,h,1.0,h,
26	1.0e-6,1.0e-6,1.0e-6,
27	Harmonic Mean,Harmonic Mean,Harmonic Mean,Harmonic Mean,
28	~Grid Geometry
29	cartesian
30	1,1,1,
31	2.1544,m,2.1544,m,2.1544,m,0.0,m,0.0,m,
32	0.0,m,
33	1 line(s) of grid geometry input follows.
34	Node 1,1.0772,m,
35	1 line(s) of grid geometry input follows.
36	Node 1,1.0772,m,
37	1 line(s) of grid geometry input follows.
38	Node 1,1.0772,m,
39	~Inactive Nodes
40	0 line(s) of inactive nodes input follows.
41	~Rock or Soil Types
42	0 character(s) of rock or soil types notes follows.
43	1 line(s) of rock or soil types input follows.
44	Generic Sand,1,1,1,1,1,1,
45	~Mechanical Properties
46	1 line(s) of mechanical properties input follows.
47	Generic Sand,0.5,0.5,0.5,,,,dependent,,,
48	~Hydraulic Properties
49	1 line(s) of hydraulic properties input follows.
50	Generic Sand,1.0E-14,1.0E-14,1.0E-14,m^2,,,,m^2,0.0,1/m,
51	~Thermal Properties
52	1 line(s) of thermal properties input follows.
53	Generic Sand,dependent,2.10,2.10,2.10,,,,W/m K,2650.0,kg/m^3,1000.0,J/kg K,
54	~Species Properties
55	0 line(s) of species properties input follows.
56	~Soil Characteristics
57	1 line(s) of soil characteristics input follows.
58	Generic Sand,van Genuchten,0.5,1/m,2.0,1.0E+8,m,,,,
59	~Liquid Relative Permeability Properties
60	1 line(s) of liquid relative permeability input follows.
61	Generic Sand,Corey's Curves,0.3,0.05,1.0E-10,,
62	~Gas Relative Permeability Properties
63	0 line(s) of gas relative permeability input follows.

Exhibit 8.3. (Contd)

Line No.	Input File
64	~Liquid Boundary Conditions
65	0 line(s) of liquid boundary conditions input follows.
66	~Gas Boundary Conditions
67	0 line(s) of gas boundary conditions input follows.
68	~Vapor Boundary Conditions
69	0 line(s) of vapor boundary conditions input follows.
70	~Energy Boundary Conditions
71	0 line(s) of energy boundary conditions input follows.
72	~Species Boundary Conditions
73	0 line(s) of species boundary conditions input follows.
74	~Initial Conditions
75	Liquid Saturation & Gas Pressure,
76	4 line(s) of initial conditions input follows.
77	Gas Pressure,4.0E+06,Pa (absolute),,1/m,,1/m,,1/m,1,1,1,1,1,1,
78	Liquid Saturation,0.0,,,1/m,,1/m,,1/m,1,1,1,1,1,1,
79	Temperature,280.0,Celsius,,1/m,,1/m,,1/m,1,1,1,1,1,1,
80	Vapor Mass Fraction,1.0,,,1/m,,1/m,,1/m,1,1,1,1,1,1,
81	~Sources & Sinks
82	1 line(s) of sources & sinks input follows.
83	Thermal Energy,Constant,-5.0E+4,W/m^3,,,,,0,s,1875.0,s,1,1,1,1,1,1,
84	~Liquid Pathline Trace
85	0 line(s) of liquid pathline trace input follows.
86	~Output Control
87	1,1,1,1,1,1,zxplane,
88	0 line(s) of output control input follows.
89	1,1,1,,,,,,,,,,1,
90	3 line(s) of output control input follows.
91	Liquid Pressure,
92	Temperature,
93	Liquid Saturation,
94	8 line(s) of output control input follows.
95	Liquid Pressure,
96	Gas Pressure,
97	Temperature,
98	Liquid Saturation,
99	Gas Phase Vapor Mass Fraction,
100	Liquid Phase Rel. Permeability,
101	Liquid Density,
102	Gas Density,
103	3 line(s) of output control input follows.
104	Liquid Pressure,
105	Temperature,
106	Liquid Saturation,
107	~Surface Flux Integrator
108	0 line(s) of surface flux integrator input follows.
109	~Rock List
110	1 line(s) of rock list input follows.
111	Generic Sand,
112	~

8.3 Flow from Hot Two-Phase Conditions

This problem is concerned with two-phase flow between two adjacent cubes of porous medium with sharply differing initial conditions. The problem starts with both nodes in two-phase conditions; however, one node is nearly saturated with relatively cool water and the other is nearly desaturated at an elevated temperature. The problem involves simulating imbibition and vaporization of the liquid water from relatively cool saturated conditions to hot dry conditions. The control volume surfaces surrounding the two nodes are adiabatic and impermeable to fluid flow. The problem proceeds until equilibrium conditions are reached. The problem demonstrates the conservation of water mass, air mass, and thermal energy for two-phase flow conditions. An energy balance error analysis is presented from the simulation results of this problem.

8.3.1 Problem Domain and Input Parameters

The problem involves two cubes of porous medium, both with porosity 0.50, volume 10 m^3, and hydraulic conductivity 1.0×10^{-14} m^2. The rock thermal conductivity, density, and specific heat are 2.10 W/m K, 2650 kg/m^3, and 1000 J/kg K, respectively. The initial conditions for the first (west) cube are: gas pressure, 1.0×10^5 Pa (absolute); liquid saturation, 0.999; temperature, 99.5°C. For the second (east) cube, the initial conditions are: gas pressure, 9.9×10^6 Pa (absolute); liquid saturation, 0.001; temperature, 310.0°C. The input file is shown in Exhibit 8.4.

8.3.2 Energy Balance Check

Let q_i represent the thermal energy in computational node i; q_i is the sum of the rock or soil internal energy, aqueous-phase-water internal energy, water-vapor internal energy, and air internal energy (the contribution from air dissolved in the aqueous phase is negligible):

$$q_i = (1-n_T)\, c_s\, \rho_s\, T + s_\ell \rho_\ell \eta_D\, u_\ell^w + s_g\, \rho_g\, x_g^w\, n_D\, u_g^w + s_g\, \rho_g \left(1-x_g^w\right) n_D\, u_g^a \tag{8.5}$$

The total energy in the problem domain at time t is the sum of all computational nodes, or Σq_i. Table 8.4 lists the values of all of the parameters required by Equation (8.5) for both initial and final conditions. All parameter values except the internal energies (u_ℓ^w, u_g^w, u_g^a) were obtained from MSTS-generated "plot" files using the "input" file shown in Exhibit 8.4. The plot file for initial conditions was obtained by changing the Initial Conditions Only option in the "input" file (Exhibit 8.4, Solution Schemes card, line 11, first option) from "false" to "true" and running MSTS again. The values for the internal energies of water in the aqueous and gas phases were

Table 8.4. Hot Two-Phase Flow Problem Initial and Final Conditions

Variable	Units	Initial Conditions		Final Conditions	
		West Node	East Node	West Node	East Node
c_s	J/kg K	1000.0	1000.0	1000.0	1000.0
n_T	-	0.50	0.50	0.50	0.50
ρ_s	kg/m³	2650.0	2650.0	2650.0	2650.0
ρ_ℓ	kg/m³	958.48	690.68	898.49	898.49
ρ_g	kg/m³	0.59213	54.724	4.2060	4.2060
s_ℓ	-	0.999	0.001	0.56160	0.56160
s_g	-	0.001	0.999	0.43840	0.43840
T	°C	99.5	310.0	168.83	168.83
u_ℓ^w	kJ/kg	416.83	1387.1	713.24	713.24
u_g^w	kJ/kg	2505.91	2546.4	2575.56	2575.56
u_g^a	kJ/kg	266.39	421.96	316.79	316.79
x_g^w	-	0.99290	0.99686	0.95439	0.95439

obtained from steam tables (Table A.1, van Wylen and Sonntag 1985). The values for the internal energy of air in the gas phase were obtained from a table of ideal gas integrals for air (Table A.10, van Wylen and Sonntag 1985).

Computing the total internal energy per unit volume for the west node at initial conditions:

$$
\begin{aligned}
q_{west}^{init} = {} & (1-0.50)\left(1000\,\frac{\mathrm{J}}{\mathrm{kg\,K}}\right)\left(2650\,\frac{\mathrm{kg}}{\mathrm{m}^3}\right)(372.65\ \mathrm{K}) \\
& + (0.999)\left(958.48\,\frac{\mathrm{kg}}{\mathrm{m}^3}\right)(0.50)\left(416{,}830\,\frac{\mathrm{J}}{\mathrm{kg}}\right) \\
& + (0.001)\left(0.59213\,\frac{\mathrm{kg}}{\mathrm{m}^3}\right)(0.99290)\,(0.50)\left(2{,}505{,}910\,\frac{\mathrm{J}}{\mathrm{kg}}\right) \\
& + (0.001)\left(0.59213\,\frac{\mathrm{kg}}{\mathrm{m}^3}\right)(1-0.99290)\,(0.50)\left(266{,}390\,\frac{\mathrm{J}}{\mathrm{kg}}\right) \\
= {} & 6.9332 \times 10^8\ \mathrm{J/m^3}
\end{aligned}
$$

which, when multiplied by the node volume (10 m^3), yields the total node energy at time zero of 6.9332×10^9 J. Repeating for the east node, we obtain

$$
\begin{aligned}
q^{init}_{east} = & (1-0.50)\left(1000\,\frac{J}{kg\,K}\right)\left(2650\,\frac{kg}{m^3}\right)(583.15\ K) \\
& + (0.001)\left(690.68\,\frac{kg}{m^3}\right)(0.50)\left(1{,}387{,}100\,\frac{J}{kg}\right) \\
& + (0.999)\left(54.724\,\frac{kg}{m^3}\right)(0.99686)\,(0.50)\left(2{,}546{,}400\,\frac{J}{kg}\right) \\
& + (0.999)\left(54.724\,\frac{kg}{m^3}\right)(1-0.99686)\,(0.50)\left(421{,}960\,\frac{J}{kg}\right) \\
= & \ 8.4258 \times 10^8\ J/m^3
\end{aligned}
$$

for which the total energy is therefore 8.4258×10^9 J. The total energy in the problem domain is the sum of these two nodes, or 15,359.0 MJ. For the final conditions, the two nodes are in equilibrium; hence only one calculation is necessary:

$$
\begin{aligned}
q^{final} = & (1-0.50)\left(1000\,\frac{J}{kg\,K}\right)\left(2650\,\frac{kg}{m^3}\right)(441.98\ K) \\
& + (0.56160)\left(898.49\,\frac{kg}{m^3}\right)(0.50)\left(713{,}240\,\frac{J}{kg}\right) \\
& + (0.43840)\left(4.2060\,\frac{kg}{m^3}\right)(0.95439)\,(0.50)\left(2{,}575{,}560\,\frac{J}{kg}\right) \\
& + (0.43840)\left(4.2060\,\frac{kg}{m^3}\right)(1-0.95439)\,(0.50)\left(316{,}790\,\frac{J}{kg}\right) \\
= & \ 7.6785 \times 10^8\ J/m^3
\end{aligned}
$$

This applies for both nodes, or a total volume of 20 m^3; hence the total energy in the system predicted by MSTS at the end of the simulation for equilibrium conditions is 15,357.0 MJ. The difference between the total energy in the domain at the beginning and at the end of the simulation (2.0 MJ) is the error introduced during the simulation by MSTS through numerical approximation, and is equal to 0.013% of the initial total energy.

Exhibit 8.4. MSTS Input File for Hot Two-Phase Problem

Line No.	Input File
1	~Simulation Title and Notes
2	beta,0001,
3	Flow from hot two-phase conditions
4	L.E. Peele
5	Battelle, Pacific Northwest Laboratory
6	Thursday, July 16, 1992
7	10:08:19 AM
8	34 character(s) of simulation title notes follows.
9	Flow from hot two-phase conditions
10	~Solution Schemes
11	false,false,false,
12	banded matrix
13	true,true,true,false,
14	1.875E+8,s,
15	10.0,s,
16	1.1,
17	1.875E+8,s,
18	true,true,false,true,true,false,
19	false,false,false,false,
20	~Numerical Control
21	8,Maximum Residual,
22	1.0,h,1.0,h,
23	1.0e-6,1.0e-6,1.0e-6,
24	Geometric Mean,Geometric Mean,Geometric Mean,Geometric Mean,
25	~Grid Geometry
26	cartesian
27	2,1,1,
28	4.3088,m,2.1544,m,2.1544,m,0.0,m,0.0,m,
29	0.0,m,
30	2 line(s) of grid geometry input follows.
31	Node 1,1.0772,m,
32	Node 2,3.2316,m,
33	1 line(s) of grid geometry input follows.
34	Node 1,1.0772,m,
35	1 line(s) of grid geometry input follows.
36	Node 1,1.0772,m,
37	~Inactive Nodes
38	0 line(s) of inactive nodes input follows.
39	~Rock or Soil Types
40	0 character(s) of rock or soil types notes follows.
41	1 line(s) of rock or soil types input follows.
42	Generic Sand,1,1,1,1,1,1,
43	~Mechanical Properties
44	1 line(s) of mechanical properties input follows.
45	Generic Sand,0.5,0.5,0.5,,,,constant,1.0,1.0,
46	~Hydraulic Properties
47	1 line(s) of hydraulic properties input follows.
48	Generic Sand,1.0E-14,1.0E-14,1.0E-14,m^2,,,,m^2,0.0,1/m,
49	~Thermal Properties
50	1 line(s) of thermal properties input follows.
51	Generic Sand,dependent,2.10,2.10,2.10,,,,W/m K,2650.0,kg/m^3,1000.0,J/kg K,
52	~Species Properties
53	0 line(s) of species properties input follows.
54	~Soil Characteristics
55	1 line(s) of soil characteristics input follows.
56	Generic Sand,van Genuchten,5.67E-01,1/m,1.798,1.0E+20,m,,,,
57	~Liquid Relative Permeability Properties
58	1 line(s) of liquid relative permeability input follows.
59	Generic Sand,Corey's Curves,0.0,0.0,1.0E-6,,
60	~Gas Relative Permeability Properties
61	1 line(s) of gas relative permeability input follows.
62	Generic Sand,Corey's Curves,0.0,0.0,1.0E-6,
63	~Liquid Boundary Conditions

Exhibit 8.4. (Contd)

Line No.	Input File
64	0 line(s) of liquid boundary conditions input follows.
65	~Gas Boundary Conditions
66	0 line(s) of gas boundary conditions input follows.
67	~Vapor Boundary Conditions
68	0 line(s) of vapor boundary conditions input follows.
69	~Energy Boundary Conditions
70	0 line(s) of energy boundary conditions input follows.
71	~Species Boundary Conditions
72	0 line(s) of species boundary conditions input follows.
73	~Initial Conditions
74	Liquid Saturation & Gas Pressure,
75	6 line(s) of initial conditions input follows.
76	Gas Pressure,1.0E+05,Pa (absolute),,1/m,,1/m,,1/m,1,1,1,1,1,1,
77	Gas Pressure,99.0E+05,Pa (absolute),,1/m,,1/m,,1/m,2,2,1,1,1,1,
78	Liquid Saturation,0.001,,,1/m,,1/m,,1/m,2,2,1,1,1,1,
79	Liquid Saturation,0.999,,,1/m,,1/m,,1/m,1,1,1,1,1,1,
80	Temperature,310.0,Celsius,,1/m,,1/m,,1/m,2,2,1,1,1,1,
81	Temperature,99.5,Celsius,,1/m,,1/m,,1/m,1,1,1,1,1,1,
82	~Sources & Sinks
83	0 line(s) of sources & sinks input follows.
84	~Liquid Pathline Trace
85	0 line(s) of liquid pathline trace input follows.
86	~Output Control
87	1,2,1,1,1,1,zxplane,
88	0 line(s) of output control input follows.
89	1,1,1,,,,,,,,,,1,
90	9 line(s) of output control input follows.
91	Liquid Pressure,
92	Gas Pressure,
93	Temperature,
94	Liquid Saturation,
95	Gas Saturation,
96	Liquid Phase Air Mass Fraction,
97	Gas Phase Vapor Mass Fraction,
98	Liquid Density,
99	Gas Density,
100	9 line(s) of output control input follows.
101	Liquid Pressure,
102	Gas Pressure,
103	Temperature,
104	Liquid Saturation,
105	Gas Saturation,
106	Liquid Phase Air Mass Fraction,
107	Gas Phase Vapor Mass Fraction,
108	Liquid Density,
109	Gas Density,
110	3 line(s) of output control input follows.
111	Liquid Pressure,
112	Temperature,
113	Liquid Saturation,
114	~Surface Flux Integrator
115	0 line(s) of surface flux integrator input follows.
116	~Rock List
117	1 line(s) of rock list input follows.
118	Generic Sand,
119	~

8.4 Philip's Vertical Infiltration Problem

This problem demonstrates that the MSTS code correctly computes a wetting front propagation with gravitational effects. Results obtained with MSTS are compared to those of a semi-analytic solution reported by Philip (1957).

8.4.1 Purpose

The purpose of this one-dimensional, time-dependent, unsaturated, single-phase, vertical infiltration problem is to demonstrate that MSTS correctly solves the water conservation equation for a wetting front in a semi-infinite porous medium. The problem involves a 15-cm column filled with Yolo light clay, first described by Moore (1939). The governing equation for this problem is the one-dimensional form of Richards' Equation:

$$C(\psi) = \frac{\partial \psi}{\partial t} = \frac{\partial}{\partial z}\left[k(\psi)\left(\frac{\partial \psi}{\partial z} - 1\right)\right] \tag{8.6}$$

where ψ = tension head (L)

$k(\psi)$ = unsaturated hydraulic conductivity (L t^{-1})

t = time (t)

z = distance along the vertical coordinate (L).

The specific moisture capacity $C(\psi)$ is given by

$$C(\psi) = \frac{\partial \theta}{\partial \psi} \tag{8.7}$$

where θ is the volumetric moisture content.

The analytic results used for this comparison were generated by the INFIL computer code (El-Kadi 1987) for conditions at the end of 2.0 hours of infiltration.

8.4.2 Model Domain and Input Parameters

The functional relationships used for the moisture-retention curves are described by Haverkamp et al. (1977). The formulae for these relationships are provided in Section 7.3. The parameter values used are as follows:

$\theta_s = 0.495$ saturated volumetric moisture content

$\theta_r = 0.124$ residual volumetric moisture content

$k_s = 0.04428$ saturated hydraulic conductivity (cm/h)

$\alpha = 739$ curve-fitting parameter

$\beta = 4.0$ curve-fitting parameter

$A = 124.6$ curve-fitting parameter

$B = 1.77$ curve-fitting parameter

These parameter values were entered into the Soil Characteristics card (Exhibit 8.5, lines 153-155) and Liquid Relative Permeability card (Exhibit 8.5, lines 156-158).

The initial conditions for the problem are a uniform pressure head of -601.8 cm, which corresponds to a moisture content of 0.238. The boundary conditions are saturation at the upper boundary and constant pressure at the initial value for the lower boundary. Thus, infiltration begins at time zero from the saturated upper boundary.

A total of 99 nodes are specified in the z-direction to represent the 15 cm of soil (Exhibit 8.5, lines 27-135). The distribution of these nodes was made to match those available from the INFIL computer code output, and is not precisely uniform as it would be if it were assigned by the MSTS Graphical Input's Uniform option.

Because MSTS is a multiphase code, we wish to express the the initial pressure as a pressure rather than a pressure head. To convert this, assuming standard conditions (20°C), we compute

$$\begin{aligned} P_\ell &= P_g + P_{cap} \\ &= 101{,}325 \text{ Pa} + \psi \rho_\ell g \\ &= 101{,}325 \text{ Pa} - \left[(601.8 \text{ cm})\left(\frac{1 \text{ m}}{100 \text{ cm}}\right)\right]\left(998.32 \frac{\text{kg}}{\text{m}^3}\right)\left(9.81 \frac{\text{m}}{\text{s}^2}\right) \\ &= 101{,}325 \text{ Pa} - 58{,}937.4 \text{ Pa} \\ &= 42{,}387.6 \text{ Pa} \end{aligned}$$

where P_ℓ is the liquid-phase pressure, P_g is the gas-phase (atmospheric) pressure, P_{cap} is the capillary pressure, and ψ is the tension head (negative of pressure head). This result is entered as liquid pressure for the initial conditions (Exhibit 8.5, line 177), along with the uniform gas pressure of 101,325 Pa (absolute), which is the atmospheric pressure (Exhibit 8.5, line 176).

8.4.3 Simulation Results and Comparison to Semi-Analytic Solution

The Philip's vertical infiltration problem was simulated by MSTS in 183 time steps. The input file was also modified to use the geometric mean and arithmetic mean techniques for computing internodal hydraulic conductivities. The liquid pressures predicted by MSTS for all three averaging techniques are compared to the Philip's analytical solution in Figure 8.3 in terms of liquid pressure head. Table 8.5 summarizes the relative root mean squares computed for the liquid saturation predictions of the three MSTS solutions. The *RRMS* for the harmonic mean technique achieved an "excellent" rating according to the criteria set forth in Baca and Magnuson (1990) while the *RRMS* for the geometric and arithmetic averaging techniques were rated "good."

Table 8.5. Comparison of MSTS Liquid Saturation Predictions to Philip's Semi-Analytical Solution for Vertical Infiltration of Water Into Yolo Light Clay After 2 Hours

Hydraulic Conductivity Averaging Technique	*RRMS*
Harmonic	0.0093
Geometric	0.0124
Arithmetic	0.0154

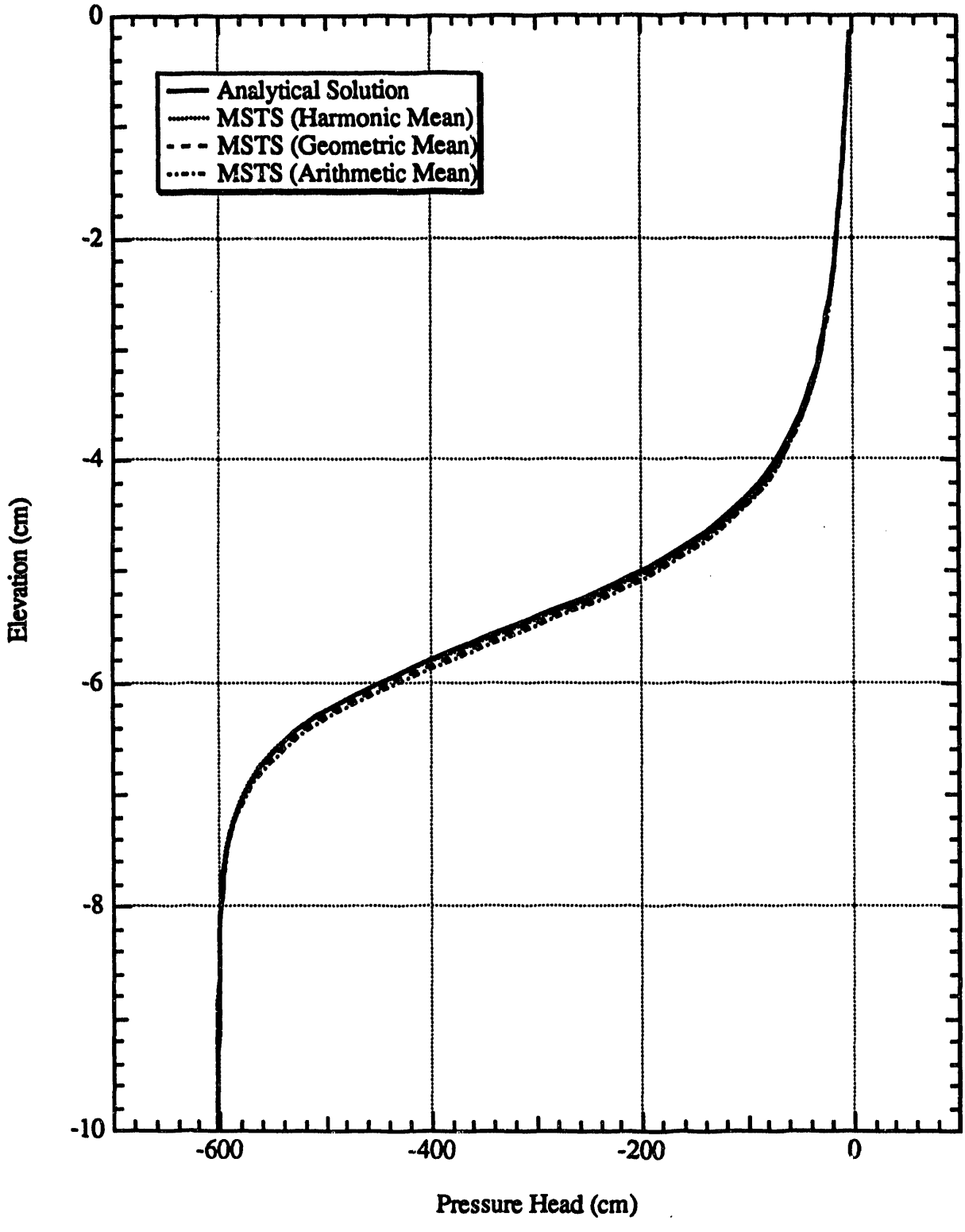

Figure 8.3. Comparison of MSTS Numerical Solutions to the Analytical Solution of the Philip's Vertical Infiltration Problem After 2 Hours of Infiltration

Exhibit 8.5. MSTS Input File for Philip's Vertical Infiltration Problem

Line No.	Input File
1	~Simulation Title and Notes
2	beta,0001,
3	Philip's Vertical Infiltration Problem
4	W. E. Nichols
5	Battelle, Pacific Northwest Laboratory
6	Monday, August 24, 1992
7	1:08:41 PM
8	200 character(s) of simulation title notes follows.
9	The objective of this test problem is to verify that the water conservation equa
10	tion of MSTS correctly computes the wetting front of the one-dimensional, time-d
11	ependent, unsaturated pressure equation.
12	~Solution Schemes
13	false,false,false,
14	banded matrix
15	false,true,false,false,
16	2.0,h,
17	0.01,h,
18	1.001,
19	0.10,h,
20	true,false,true,true,false,false,
21	false,false,false,false,
22	~Numerical Control
23	8,Maximum Residual,
24	1.0,h,1.0,h,
25	1.0E-06,1.0E-06,1.0E-06,
26	Harmonic Mean,Harmonic Mean,Harmonic Mean,Harmonic Mean,
27	~Grid Geometry
28	cartesian
29	1,1,99,
30	1,cm,1,cm,15.0,cm,0.0,cm,-15.0,cm,
31	0.0,m,
32	1 line(s) of grid geometry input follows.
33	Node 1,0.5,cm,
34	1 line(s) of grid geometry input follows.
35	Node 1,0.5,cm,
36	99 line(s) of grid geometry input follows.
37	Node 1,0.150,cm,
38	Node 2,0.300,cm,
39	Node 3,0.450,cm,
40	Node 4,0.600,cm,
41	Node 5,0.750,cm,
42	Node 6,0.900,cm,
43	Node 7,1.050,cm,
44	Node 8,1.200,cm,
45	Node 9,1.350,cm,
46	Node 10,1.500,cm,
47	Node 11,1.650,cm,
48	Node 12,1.800,cm,
49	Node 13,1.950,cm,
50	Node 14,2.100,cm,
51	Node 15,2.250,cm,
52	Node 16,2.400,cm,
53	Node 17,2.550,cm,
54	Node 18,2.700,cm,
55	Node 19,2.850,cm,
56	Node 20,3.000,cm,
57	Node 21,3.150,cm,
58	Node 22,3.300,cm,
59	Node 23,3.450,cm,
60	Node 24,3.600,cm,
61	Node 25,3.750,cm,
62	Node 26,3.900,cm,
63	Node 27,4.050,cm,

Exhibit 8.5. (Contd)

Line No.	Input File
64	Node 28,4.200,cm,
65	Node 29,4.350,cm,
66	Node 30,4.500,cm,
67	Node 31,4.650,cm,
68	Node 32,4.800,cm,
69	Node 33,4.950,cm,
70	Node 34,5.100,cm,
71	Node 35,5.250,cm,
72	Node 36,5.400,cm,
73	Node 37,5.550,cm,
74	Node 38,5.700,cm,
75	Node 39,5.850,cm,
76	Node 40,6.000,cm,
77	Node 41,6.150,cm,
78	Node 42,6.300,cm,
79	Node 43,6.450,cm,
80	Node 44,6.600,cm,
81	Node 45,6.750,cm,
82	Node 46,6.900,cm,
83	Node 47,7.050,cm,
84	Node 48,7.200,cm,
85	Node 49,7.350,cm,
86	Node 50,7.500,cm,
87	Node 51,7.650,cm,
88	Node 52,7.800,cm,
89	Node 53,7.950,cm,
90	Node 54,8.100,cm,
91	Node 55,8.250,cm,
92	Node 56,8.400,cm,
93	Node 57,8.550,cm,
94	Node 58,8.700,cm,
95	Node 59,8.850,cm,
96	Node 60,9.000,cm,
97	Node 61,9.150,cm,
98	Node 62,9.300,cm,
99	Node 63,9.450,cm,
100	Node 64,9.600,cm,
101	Node 65,9.750,cm,
102	Node 66,9.900,cm,
103	Node 67,10.050,cm,
104	Node 68,10.200,cm,
105	Node 69,10.350,cm,
106	Node 70,10.500,cm,
107	Node 71,10.650,cm,
108	Node 72,10.800,cm,
109	Node 73,10.950,cm,
110	Node 74,11.100,cm,
111	Node 75,11.250,cm,
112	Node 76,11.400,cm,
113	Node 77,11.550,cm,
114	Node 78,11.700,cm,
115	Node 79,11.850,cm,
116	Node 80,12.000,cm,
117	Node 81,12.150,cm,
118	Node 82,12.300,cm,
119	Node 83,12.450,cm,
120	Node 84,12.600,cm,
121	Node 85,12.750,cm,
122	Node 86,12.900,cm,
123	Node 87,13.050,cm,
124	Node 88,13.200,cm,
125	Node 89,13.350,cm,
126	Node 90,13.500,cm,

Exhibit 8.5. (Contd)

Line No.	Input File
127	Node 91,13.650,cm,
128	Node 92,13.800,cm,
129	Node 93,13.950,cm,
130	Node 94,14.100,cm,
131	Node 95,14.250,cm,
132	Node 96,14.400,cm,
133	Node 97,14.550,cm,
134	Node 98,14.700,cm,
135	Node 99,14.850,cm,
136	~Inactive Nodes
137	0 line(s) of inactive nodes input follows.
138	~Rock or Soil Types
139	52 character(s) of rock or soil types notes follows.
140	Yolo light clay was first described by Moore (1939).
141	1 line(s) of rock or soil types input follows.
142	Yolo Light Clay,1,1,1,1,1,99,
143	~Mechanical Properties
144	1 line(s) of mechanical properties input follows.
145	Yolo Light Clay,0.495,0.371,0.371,,,,constant,,,
146	~Hydraulic Properties
147	1 line(s) of hydraulic properties input follows.
148	Yolo Light Clay,1.2300e-7,1.2300e-7,1.2300e-7,hc:m/s,,,,m^2,0.124,1/m,
149	~Thermal Properties
150	0 line(s) of thermal properties input follows.
151	~Species Properties
152	0 line(s) of species properties input follows.
153	~Soil Characteristics
154	1 line(s) of soil characteristics input follows.
155	Yolo Light Clay,Haverkamp,739.0,,4.0,1.0E+20,m,,,,
156	~Liquid Relative Permeability Properties
157	1 line(s) of liquid relative permeability input follows.
158	Yolo Light Clay,Haverkamp,124.6,1.77,1.0E-20,,
159	~Gas Relative Permeability Properties
160	0 line(s) of gas relative permeability input follows.
161	~Liquid Boundary Conditions
162	2 line(s) of liquid boundary conditions input follows.
163	Z-Direction: Top Surface,Dirichlet @ Boundary,101325.0,Pa (absolute),998.32, kg/m^3,,1,1,1,1,99,99,
164	Z-Direction: Bottom Surface,Dirichlet @ Boundary,42387.6,Pa (absolute),998.32, kg/m^3,,1,1,1,1,1,1,
165	~Gas Boundary Conditions
166	0 line(s) of gas boundary conditions input follows.
167	~Vapor Boundary Conditions
168	0 line(s) of vapor boundary conditions input follows.
169	~Energy Boundary Conditions
170	0 line(s) of energy boundary conditions input follows.
171	~Species Boundary Conditions
172	0 line(s) of species boundary conditions input follows.
173	~Initial Conditions
174	Gas Pressure & Liquid Pressure,
175	2 line(s) of initial conditions input follows.
176	Gas Pressure,101325.0,Pa (absolute),0.0,1/m,0.0,1/m,0.0,1/m,1,1,1,1,1,99,
177	Liquid Pressure,42387.6015,Pa (absolute),0.0,1/m,0.0,1/m,0.0,1/m,1,1,1,1,1,99,
178	~Sources & Sinks
179	0 line(s) of sources & sinks input follows.
180	~Liquid Pathline Trace
181	0 line(s) of liquid pathline trace input follows.
182	~Output Control
183	1,1,1,1,1,99,zxplane,
184	1 line(s) of output control input follows.
185	2.0,h,
186	1,1,90,1,1,80,1,1,70,1,1,60,1,
187	0 line(s) of output control input follows.

Exhibit 8.5. (Contd)

Line No.	Input File
157	6 line(s) of output control input follows.
158	Liquid Pressure,
159	Liquid Saturation,
160	Liquid Phase Rel. Permeability,
161	Total Hydraulic Head,
162	Volumetric Moisture Content,
163	Z-Dir. Liquid Velocity,
164	5 line(s) of output control input follows.
165	Liquid Pressure,
166	Liquid Saturation,
167	Total Hydraulic Head,
168	Volumetric Moisture Content,
169	Z-Dir. Liquid Velocity,
170	~Surface Flux Integrator
171	0 line(s) of surface flux integrator input follows.
172	~Rock List
173	1 line(s) of rock list input follows.
174	Yolo Light Clay,
175	~

8.5 Two-Dimensional Infiltration

This is a two-dimensional infiltration problem proposed by Ross et al. (1982) that is concerned with liquid flow through a two-dimensional rectangular section (10 cm high by 15 cm wide) of partially saturated soil with uniform initial conditions. A wetting surface is propagated through the domain by imposing a wetting surface on a portion of a boundary and allowing the water introduced at the boundary to infiltrate over time. The purpose of the problem is to demonstrate how MSTS propagates a wetting front in two dimensions with gravitational effects.

8.5.1 Problem Domain and Input Parameters

The top 4 cm of the left boundary is maintained at a prescribed capillary (tension) head of $-\psi = 6 - z$ (6 cm $\leq z \leq$ 10 cm). The whole right boundary is maintained at a prescribed capillary (tension) head of $-\psi = 90$ cm. All other boundary surfaces are defined as zero-flux surfaces. Figure 8.4 provides a schematic of the problem and illustrates the discretization and boundary condition placement (unmarked boundaries are zero-flux).

The input file for this problem is shown in Exhibit 8.6. The soil-moisture tension characteristic and relative-permeability curves for the soil are provided as tabular input; these are shown graphically in Figure 8.5.

8.5.2 Simulation Results

Figure 8.6 shows two capillary pressure profiles, along the top ($z = 9.5$ cm) and the bottom ($z = 0.5$ cm) of the domain at the same time. Figure 8.7 shows the liquid saturation contours for the domain at the end of the simulation at time 0.508 day. Ross et al. (1982) only proposed this problem; they did not provide a solution (it had not yet been simulated). Pruess (1987) demonstrated the solution to this problem using the TOUGH code. The results reported here are essentially the same as those reported by Pruess (1987).

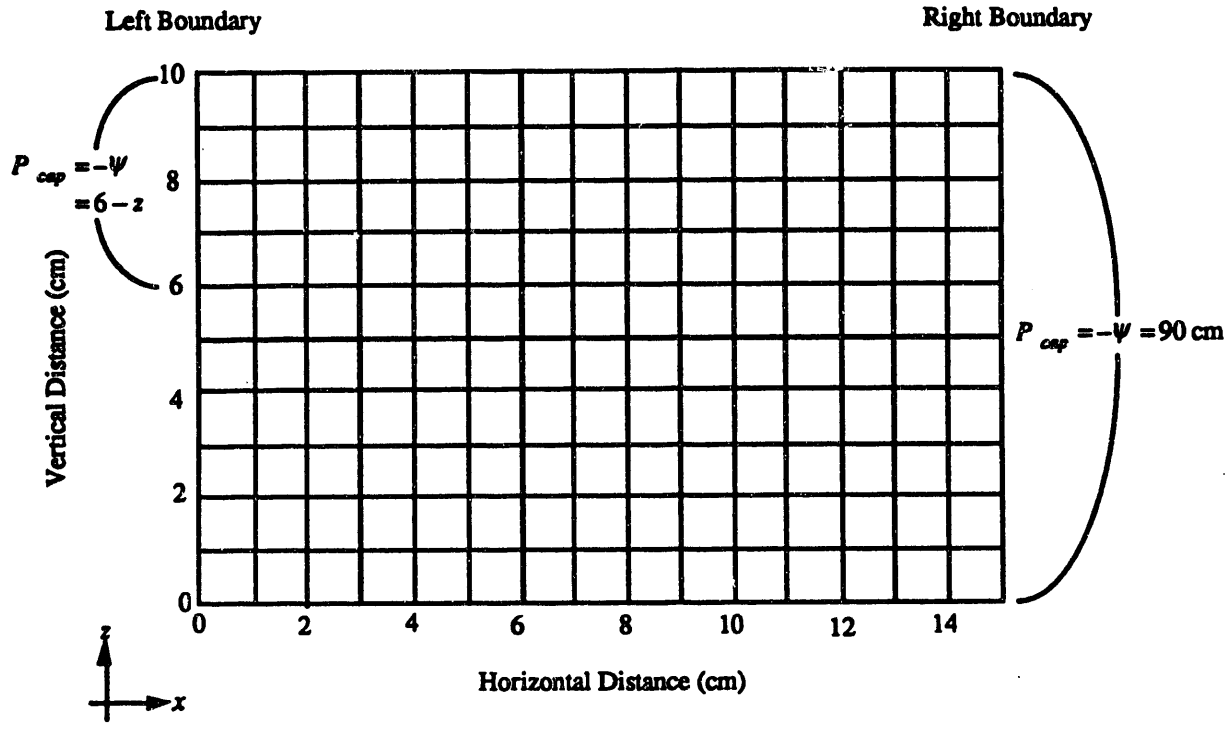

Figure 8.4. Two-Dimensional Infiltration Problem Geometry, Discretization, and Boundary Conditions

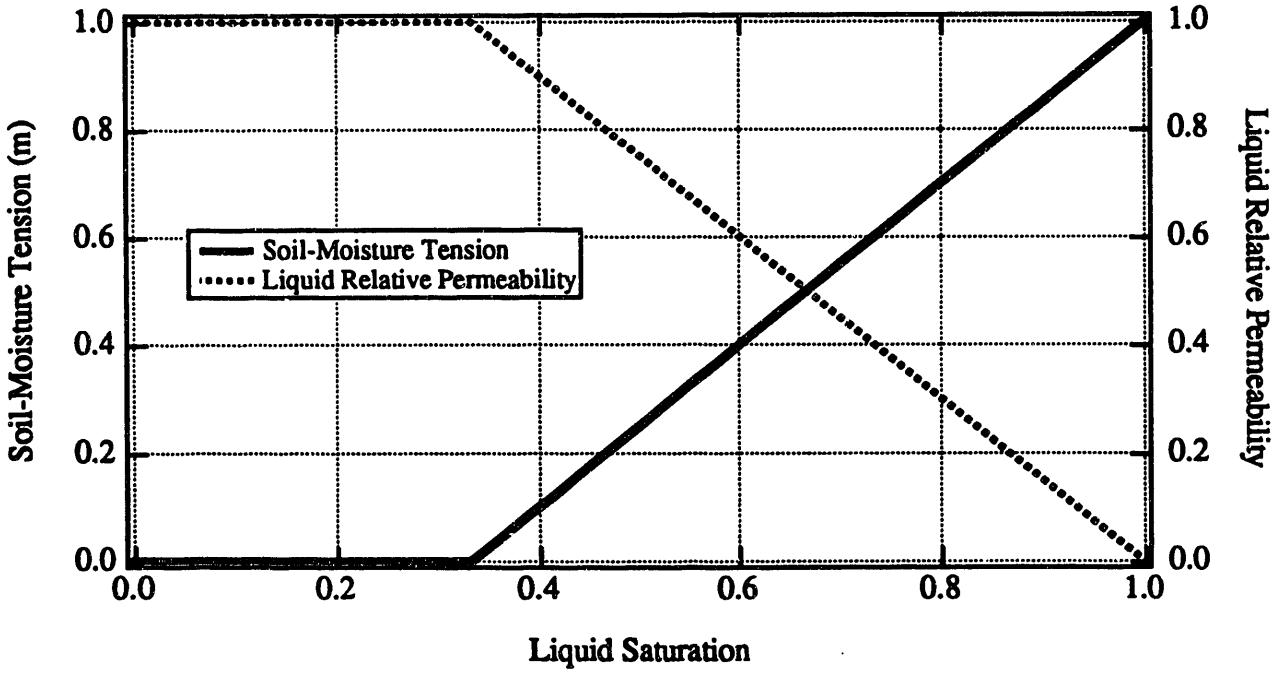

Figure 8.5. Functional Relationships Among Liquid Saturation, Liquid Pressure, and Liquid Relative Permeability for the Two-Dimensional Infiltration Problem

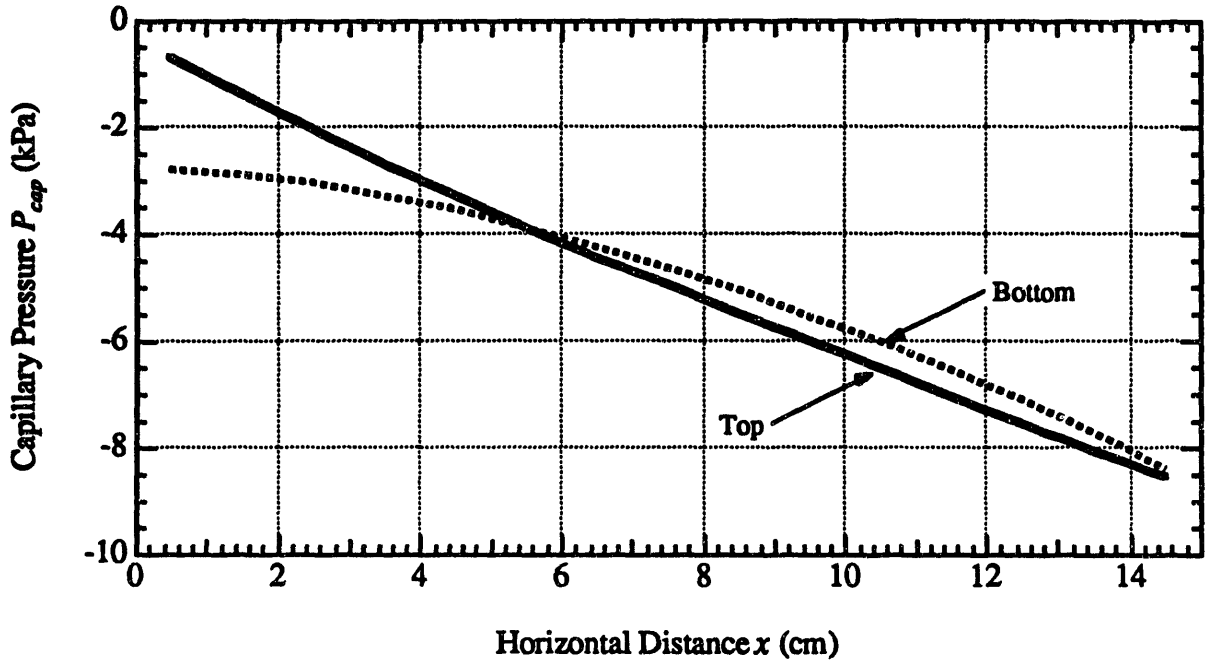

Figure 8.6. Capillary Pressure Profiles at 0.508 Day for Two-Dimensional Infiltration Problem

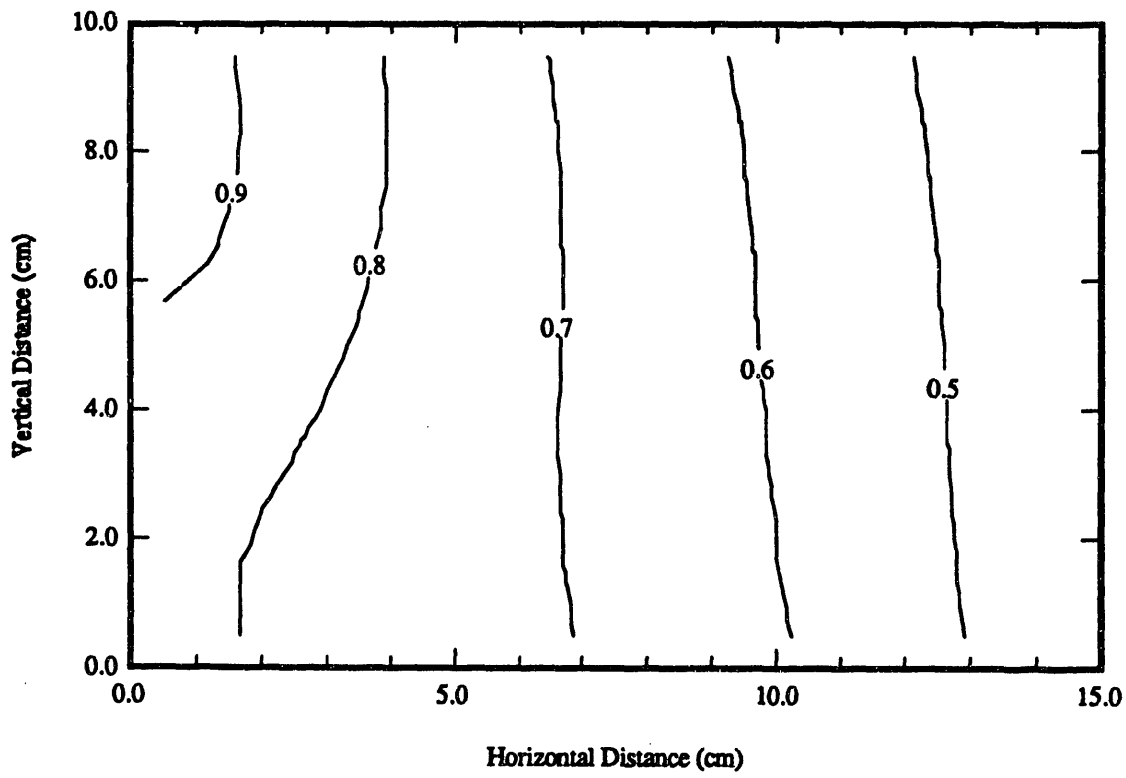

Figure 8.7. Liquid Saturation Contours at 0.508 Day for Two-Dimensional Infiltration Problem

Exhibit 8.6. MSTS Input File for Two-Dimensional Infiltration Problem

Line No.	Input File
1	~Simulation Title and Notes
2	beta,0001,
3	Two-Dimensional Infiltration With Gravity
4	W. E. Nichols
5	Battelle, Pacific Northwest Laboratory
6	Thursday, August 27, 1992
7	1:05:00 PM
8	94 character(s) of simulation title notes follows.
9	Two-dimensional infiltration into a column of soil 10 centimeters high by 15 cen
10	timeters wide.
11	~Solution Schemes
12	false,false,false,
13	banded matrix
14	false,true,false,false,
15	0.508,day,
16	0.001,day,
17	1.25,
18	0.508,day,
19	true,false,true,true,false,false,
20	false,false,false,false,
21	~Numerical Control
22	8,Maximum Residual,
23	2.0,h,2.0,h,
24	1.0E-06,1.0E-06,1.0E-06,
25	Harmonic Mean,Harmonic Mean,Harmonic Mean,Harmonic Mean,
26	~Grid Geometry
27	cartesian
28	15,1,10,
29	15.0,cm,1.0,cm,10.0,cm,0.0,cm,0.0,cm,
30	0.0,m,
31	15 line(s) of grid geometry input follows.
32	Node 1,0.5,cm,
33	Node 2,1.5,cm,
34	Node 3,2.5,cm,
35	Node 4,3.5,cm,
36	Node 5,4.5,cm,
37	Node 6,5.5,cm,
38	Node 7,6.5,cm,
39	Node 8,7.5,cm,
40	Node 9,8.5,cm,
41	Node 10,9.5,cm,
42	Node 11,10.5,cm,
43	Node 12,11.5,cm,
44	Node 13,12.5,cm,
45	Node 14,13.5,cm,
46	Node 15,14.5,cm,
47	1 line(s) of grid geometry input follows.
48	Node 1,0.5,cm,
49	10 line(s) of grid geometry input follows.
50	Node 1,0.5,cm,
51	Node 2,1.5,cm,
52	Node 3,2.5,cm,
53	Node 4,3.5,cm,
54	Node 5,4.5,cm,
55	Node 6,5.5,cm,
56	Node 7,6.5,cm,
57	Node 8,7.5,cm,
58	Node 9,8.5,cm,
59	Node 10,9.5,cm,
60	~Inactive Nodes
61	0 line(s) of inactive nodes input follows.
62	~Rock or Soil Types
63	33 character(s) of rock or soil types notes follows.

Exhibit 8.6. (Contd)

Line No.	Input File
64	Problem 4.2 of Ross et al. (1982)
65	1 line(s) of rock or soil types input follows.
66	Homogeneous Soil,1,15,1,1,1,10,
67	~Mechanical Properties
68	1 line(s) of mechanical properties input follows.
69	Homogeneous Soil,0.45,0.45,0.30,,,,dependent,,,
70	~Hydraulic Properties
71	1 line(s) of hydraulic properties input follows.
72	Homogeneous Soil,1.2E-14,1.2E-14,1.2E-14,m^2,,,,m^2,1.9,1/m,
73	~Thermal Properties
74	1 line(s) of thermal properties input follows.
75	Homogeneous Soil,independent,1.0e+5,1.0e+5,1.0e+5,1.0e+5,1.0e+5,1.0e+5,W/m K, 2385,kg/m^3,1030,J/kg K,
76	~Species Properties
77	0 line(s) of species properties input follows.
78	~Soil Characteristics
79	1 line(s) of soil characteristics input follows.
80	Homogeneous Soil,Tabular,Table No. 1,
81	2 line(s) of capillary tables input follows.
82	0.0,1.0,m,
83	1.0,0.333,m,
84	~Liquid Relative Permeability Properties
85	1 line(s) of liquid relative permeability input follows.
86	Homogeneous Soil,Tabular vs Liquid Saturation,Table No. 1,
87	3 line(s) of liquid permeability tables input follows.
88	0.0,0.0,
89	0.333,0.0,
90	1.0,1.0,
91	~Gas Relative Permeability Properties
92	1 line(s) of gas relative permeability input follows.
93	Homogeneous Soil,Tabular vs Liquid Saturation,Table No. 1,
94	2 line(s) of gas permeability tables input follows.
95	0.0,1.0,
96	1.0,1.0,
97	~Liquid Boundary Conditions
98	5 line(s) of liquid boundary conditions input follows.
99	X-Direction: West Surface,Dirichlet @ Boundary,101276.06,Pa (absolute),998.32, kg/m^3,,1,1,1,1,7,7,
100	X-Direction: West Surface,Dirichlet @ Boundary,101178.17,Pa (absolute),998.32, kg/m^3,,1,1,1,1,8,8,
101	X-Direction: West Surface,Dirichlet @ Boundary,101080.28,Pa (absolute),998.32, kg/m^3,,1,1,1,1,9,9,
102	X-Direction: West Surface,Dirichlet @ Boundary,100982.39,Pa (absolute),998.32, kg/m^3,,1,1,1,1,10,10,
103	X-Direction: East Surface,Dirichlet @ Boundary,92514.90,Pa (absolute),998.32, kg/m^3,,15,15,1,1,1,10,
104	~Gas Boundary Conditions
105	0 line(s) of gas boundary conditions input follows.
106	~Vapor Boundary Conditions
107	0 line(s) of vapor boundary conditions input follows.
108	~Energy Boundary Conditions
109	0 line(s) of energy boundary conditions input follows.
110	~Species Boundary Conditions
111	0 line(s) of species boundary conditions input follows.
112	~Initial Conditions
113	Liquid Saturation & Gas Pressure,
114	2 line(s) of initial conditions input follows.
115	Gas Pressure,101325.0,Pa (absolute),,1/m,,1/m,,1/m,1,15,1,1,1,10,
116	Liquid Saturation,0.3333,,,1/m,,1/m,,1/m,1,15,1,1,1,10,
117	~Sources & Sinks
118	0 line(s) of sources & sinks input follows.
119	~Liquid Pathline Trace
120	0 line(s) of liquid pathline trace input follows.

Exhibit 8.6. (Contd)

Line No.	Input File
121	~Output Control
122	1,15,1,1,1,10,zxplane,
123	1 line(s) of output control input follows.
124	0.508,day,
125	5,1,2,5,1,9,10,1,2,10,1,9,1,
126	6 line(s) of output control input follows.
127	Liquid Pressure,
128	Liquid Saturation,
129	Liquid Phase Rel. Permeability,
130	Volumetric Moisture Content,
131	X-Dir. Liquid Velocity,
132	Z-Dir. Liquid Velocity,
133	6 line(s) of output control input follows.
134	Liquid Pressure,
135	Liquid Saturation,
136	Liquid Phase Rel. Permeability,
137	Volumetric Moisture Content,
138	X-Dir. Liquid Velocity,
139	Z-Dir. Liquid Velocity,
140	5 line(s) of output control input follows.
141	Liquid Pressure,
142	Liquid Saturation,
143	Liquid Phase Rel. Permeability,
144	X-Dir. Liquid Velocity,
145	Z-Dir. Liquid Velocity,
146	~Surface Flux Integrator
147	0 line(s) of surface flux integrator input follows.
148	~Rock List
149	1 line(s) of rock list input follows.
150	Homogeneous Soil,
151	~

8.6 One-Dimensional Two-Phase Infiltration

Touma and Vauclin (1986) demonstrated, both experimentally and numerically, the effects of air flow on water infiltration in a 93.5-cm column of soil. Touma and Vauclin (1986) applied three types of boundary conditions to the top of the soil column: 1) positive time–constant liquid head, 2) positive time–constant liquid flux less than the saturated soil hydraulic conductivity, and 3) positive time–constant liquid flux greater than the saturated hydraulic conductivity. In this section, the positive time–constant liquid head (referred to as ponded infiltration) simulations of Touma and Vauclin (1986) are repeated using MSTS to demonstrate the impact of air flow on water infiltration rates. Two simulations are described: one for a column open to air flow at the base, and one closed at the base so that air must flow out the top as water infiltrates.

8.6.1 Problem Domain and Input Parameters

The problem domain is a column of soil of height $L = 93.5$ cm for which hydraulic properties were experimentally determined by Touma and Vauclin (1986). The experimental data for the relationship between capillary pressure head and water content were statistically fit by Touma and Vauclin (1986) with the van Genuchten analytical expression (van Genuchten 1980). No distinction was made between drainage and infiltration in this expression (i.e., hysteresis was not modeled). The relationships between soil-moisture tension and liquid saturation used in the MSTS simulation are shown in Figure 8.8a. The relationships between air and water relative permeability and liquid saturation were experimentally determined and are shown in Figure 8.8b.

The first case is the open column, which represents the traditional single-phase solution for water infiltration neglecting air-flow effects. The MSTS input file for this problem is provided in Exhibit 8.7. The Water mode (Section 2.4.1) is used in this solution. The upper boundary is specified as a Dirichlet condition equivalent to a constant hydraulic head of 2.3 cm while the lower boundary is specified as a Dirichlet condition equal to the initial condition (Exhibit 8.7, Liquid Boundary Conditions card, lines 157-160). Touma and Vauclin (1986) specified that the initial condition of the soil column was reached by draining the saturated column to the static equilibrium corresponding to a piezometric level at 120 cm below the surface (top) of the column. The initial hydrologic conditions are specified as a uniform gas pressure of 101,325 Pa and a liquid pressure that is computed directly from the van Genuchten relation for a zero hydraulic gradient (pressure head and elevation head equal throughout). Examine the actual input card (Exhibit 8.7, Initial Conditions card, lines 169-173) to see how the input condition is specified using the gradient feature of the Initial Conditions card.

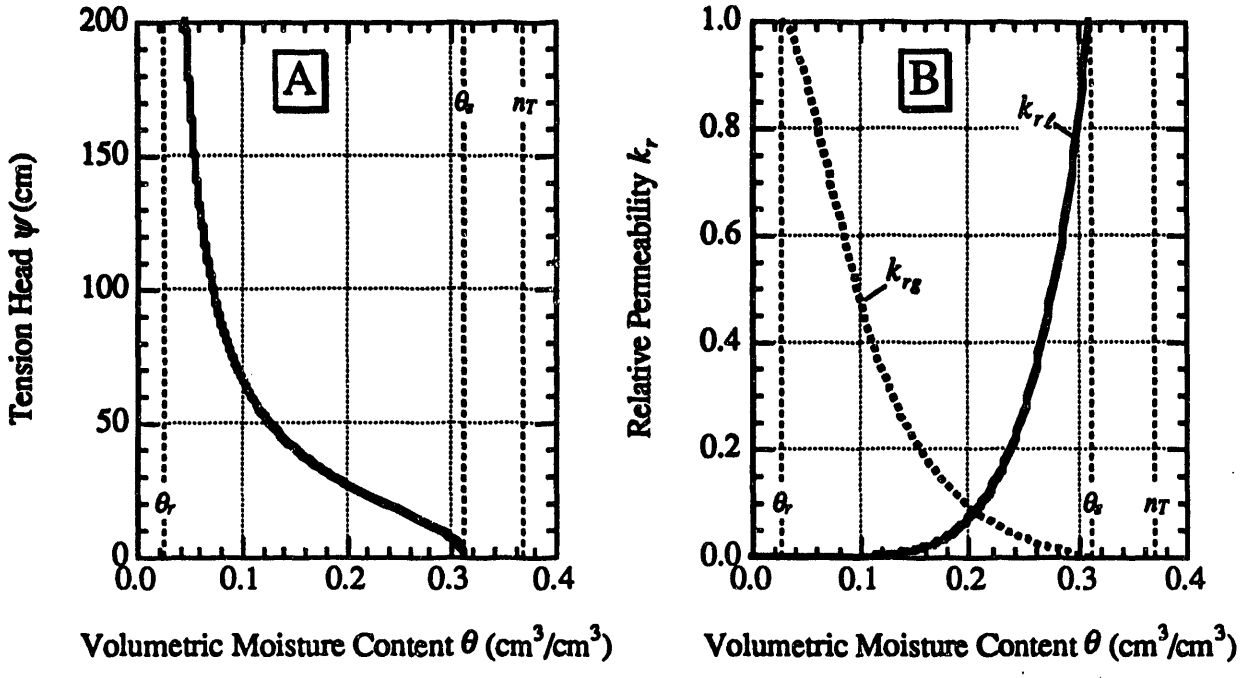

Figure 8.8. Moisture-Retention and Relative-Permeability Functions for the One-Dimensional Two-Phase Infiltration Problem: A) Relationship Between Volumetric Moisture Content and Tension Head, B) Relationship Between Volumetric Moisture Content and Liquid and Gas Relative Permeabilities

The second simulation includes the effects of air flow in the column. The Water-Air mode (Section 2.4.3) is used and the gas boundary conditions are defined to address this issue. Exhibit 8.8 shows the MSTS input file for this simulation. A longer time is simulated than for the open column case (1.2 hour rather than 0.4 hour) because the inclusion of air flow slows the wetting front greatly, as reported by Touma and Vauclin (1986). Touma and Vauclin also reported that the air-entry pressure was estimated to be 14 cm for this problem. Hence, the gas pressure at the upper boundary is specified as the pressure equivalent of the liquid pressure boundary (2.3 cm) plus the air-entry pressure (14.0 cm), or 101,550.25 Pa (Exhibit 8.8, Gas Boundary Conditions card, lines 161-164).

8.6.2 Simulation Results

The water content profiles for the open-column case, which represents traditional single-phase infiltration models, are depicted in Figure 8.9. The water content profiles for the bounded-column case are depicted in Figure 8.10. Comparing the two figures, we observe as Touma and Vauclin (1986) reported that the rate of advance of the wetting front is drastically reduced when air cannot escape. Notice also the reduction in the maximum saturation of the water content profiles

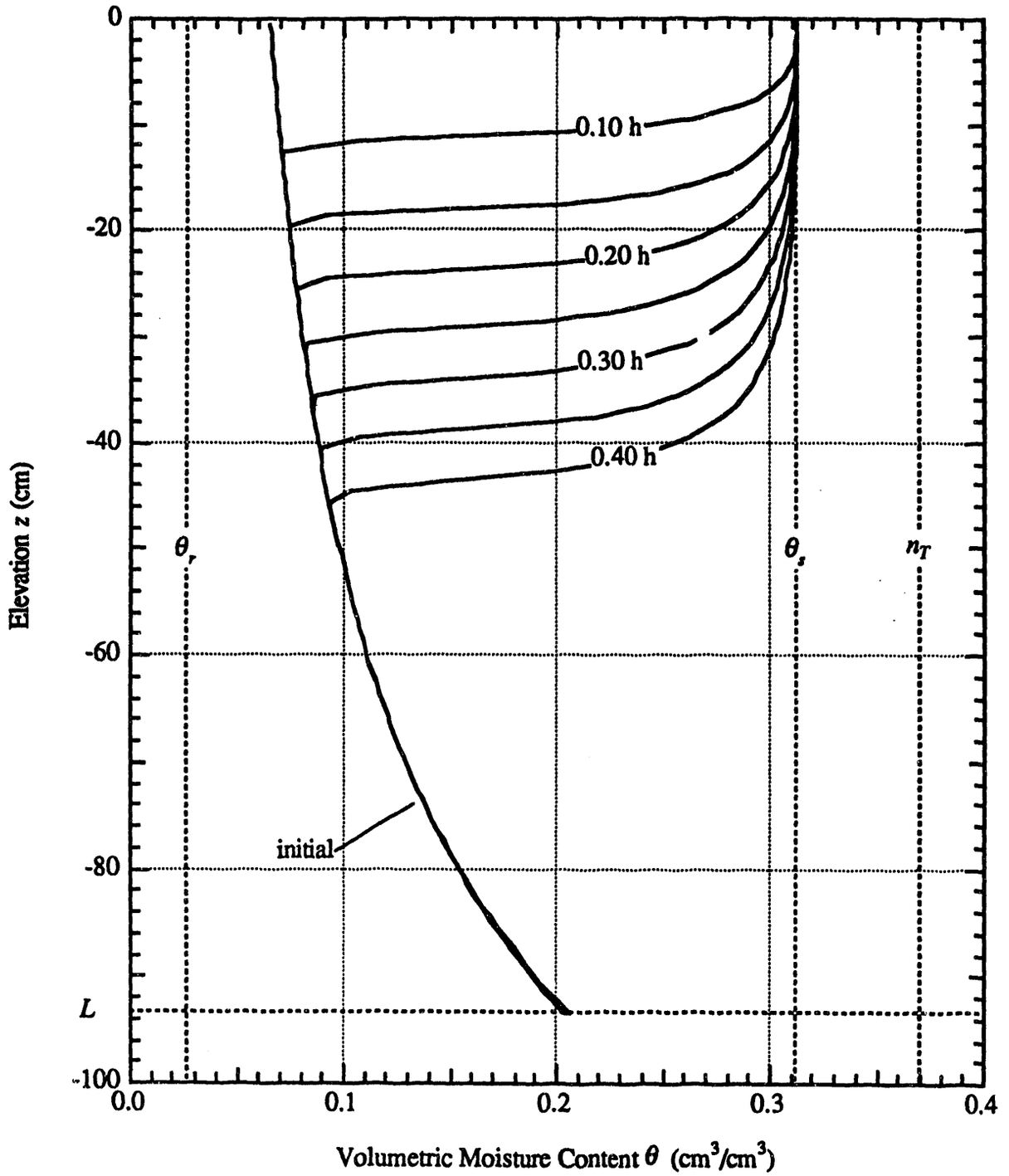

Figure 8.9. Water Content Profiles Predicted by MSTS for Ponded Infiltration in the One-Dimensional, Two-Phase Infiltration Problem: Open Column

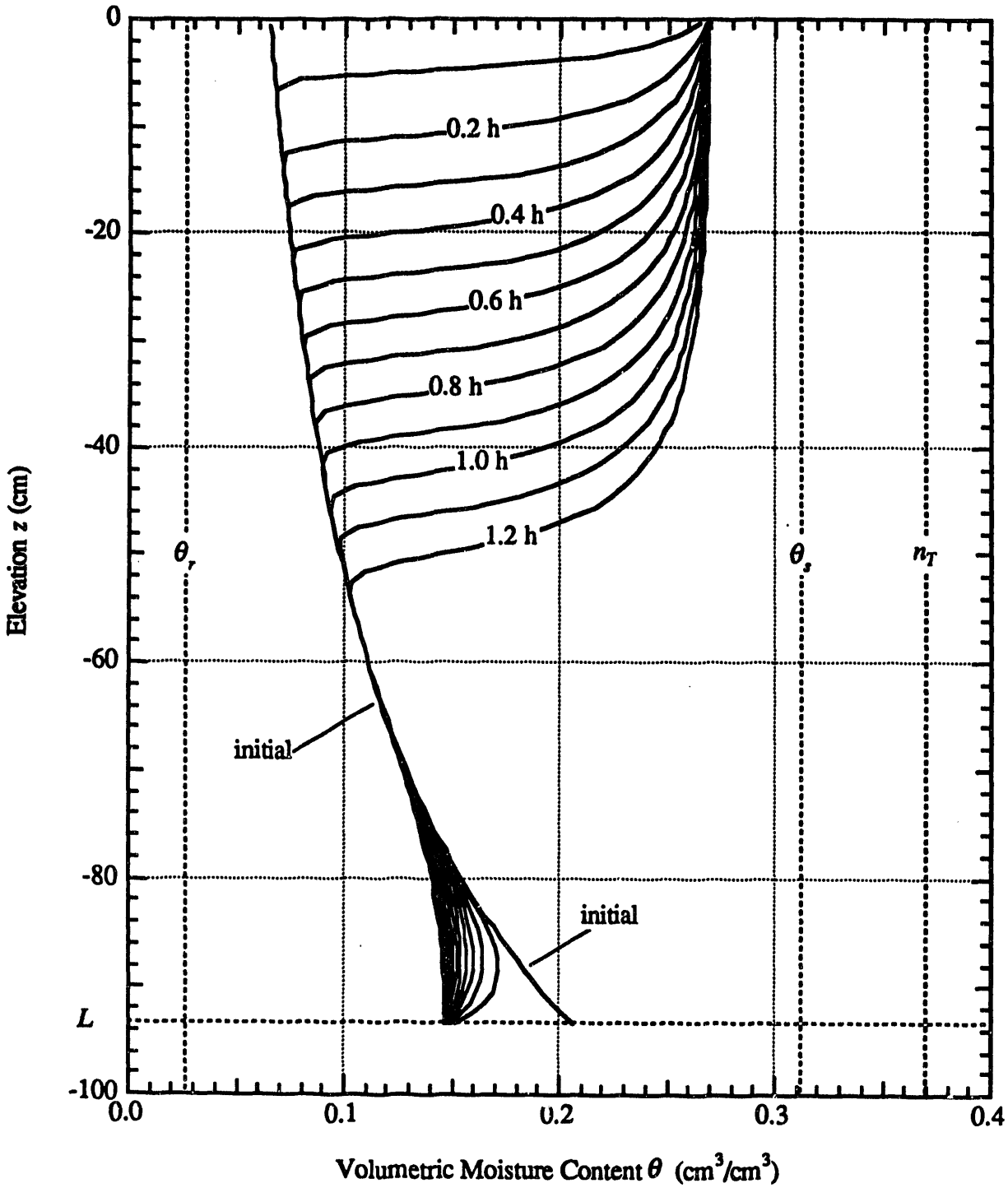

Figure 8.10. Water Content Profiles Predicted by MSTS for Ponded Infiltration in the One-Dimensional, Two-Phase Infiltration Problem: Bounded Column

from 0.312 cm^3/cm^3 in the open-column case to approximately 0.27 cm^3/cm^3 in the bounded-column case, an effect caused by the flow of escaping air. Finally, we note that the wetting fronts shown in Figure 8.10 for the bounded-column case are less steep than for the open-column case shown in Figure 8.9.

Exhibit 8.7. MSTS Input File for Two-Phase Infiltration Problem, Open Column

Line No. **Input File**

```
 1  ~Simulation Title and Notes
 2  beta,0001,
 3  1D Ponded Boundary Infiltration in Open Column
 4  W. E. Nichols
 5  Battelle, Pacific Northwest Laboratory
 6  Tuesday, October 6, 1992
 7  3:24:00 PM
 8  225 character(s) of simulation title notes follows.
 9  Simulation of infiltration in an open column after numerical and experimental re
10  sults reported in Touma and Vauclin (1986).  Initial conditions are computed fro
11  m the zero-hydraulic-gradient condition.  The Water mode is used.
12  ~Solution Schemes
13  false,false,false,
14  banded matrix
15  false,true,false,false,
16  0.40,h,
17  0.0001,h,
18  1.5,
19  0.005,h,
20  true,false,true,true,false,false,
21  false,false,false,false,
22  ~Numerical Control
23  8,Maximum Residual,
24  1.0,h,1.0,h,
25  1.0E-06,1.0E-06,1.0E-06,
26  Geometric Mean,Geometric Mean,Geometric Mean,Geometric Mean,
27  ~Grid Geometry
28  cartesian
29  1,1,94,
30  1.0,cm,1.0,cm,94.0,cm,0.0,cm,-94.0,cm,
31  0.0,cm,
32  1 line(s) of grid geometry input follows.
33  Node 1,0.5,cm,
34  1 line(s) of grid geometry input follows.
35  Node 1,0.5,cm,
36  94 line(s) of grid geometry input follows.
37  Node 1,0.5,cm,
38  Node  2,1.5,cm,
39  Node  3,2.5,cm,
40  Node  4,3.5,cm,
41  Node  5,4.5,cm,
42  Node  6,5.5,cm,
43  Node  7,6.5,cm,
44  Node  8,7.5,cm,
45  Node  9,8.5,cm,
46  Node  10,9.5,cm,
47  Node  11,10.5,cm,
48  Node  12,11.5,cm,
49  Node  13,12.5,cm,
50  Node  14,13.5,cm,
51  Node  15,14.5,cm,
52  Node  16,15.5,cm,
53  Node  17,16.5,cm,
54  Node  18,17.5,cm,
55  Node  19,18.5,cm,
56  Node  20,19.5,cm,
57  Node  21,20.5,cm,
58  Node  22,21.5,cm,
59  Node  23,22.5,cm,
60  Node  24,23.5,cm,
61  Node  25,24.5,cm,
62  Node  26,25.5,cm,
63  Node  27,26.5,cm,
```

Exhibit 8.7. (Contd)

Line No.	Input File
64	Node 28,27.5,cm,
65	Node 29,28.5,cm,
66	Node 30,29.5,cm,
67	Node 31,30.5,cm,
68	Node 32,31.5,cm,
69	Node 33,32.5,cm,
70	Node 34,33.5,cm,
71	Node 35,34.5,cm,
72	Node 36,35.5,cm,
73	Node 37,36.5,cm,
74	Node 38,37.5,cm,
75	Node 39,38.5,cm,
76	Node 40,39.5,cm,
77	Node 41,40.5,cm,
78	Node 42,41.5,cm,
79	Node 43,42.5,cm,
80	Node 44,43.5,cm,
81	Node 45,44.5,cm,
82	Node 46,45.5,cm,
83	Node 47,46.5,cm,
84	Node 48,47.5,cm,
85	Node 49,48.5,cm,
86	Node 50,49.5,cm,
87	Node 51,50.5,cm,
88	Node 52,51.5,cm,
89	Node 53,52.5,cm,
90	Node 54,53.5,cm,
91	Node 55,54.5,cm,
92	Node 56,55.5,cm,
93	Node 57,56.5,cm,
94	Node 58,57.5,cm,
95	Node 59,58.5,cm,
96	Node 60,59.5,cm,
97	Node 61,60.5,cm,
98	Node 62,61.5,cm,
99	Node 63,62.5,cm,
100	Node 64,63.5,cm,
101	Node 65,64.5,cm,
102	Node 66,65.5,cm,
103	Node 67,66.5,cm,
104	Node 68,67.5,cm,
105	Node 69,68.5,cm,
106	Node 70,69.5,cm,
107	Node 71,70.5,cm,
108	Node 72,71.5,cm,
109	Node 73,72.5,cm,
110	Node 74,73.5,cm,
111	Node 75,74.5,cm,
112	Node 76,75.5,cm,
113	Node 77,76.5,cm,
114	Node 78,77.5,cm,
115	Node 79,78.5,cm,
116	Node 80,79.5,cm,
117	Node 81,80.5,cm,
118	Node 82,81.5,cm,
119	Node 83,82.5,cm,
120	Node 84,83.5,cm,
121	Node 85,84.5,cm,
122	Node 86,85.5,cm,
123	Node 87,86.5,cm,
124	Node 88,87.5,cm,
125	Node 89,88.5,cm,
126	Node 90,89.5,cm,

Exhibit 8.7. (Contd)

Line No.	Input File
127	Node 91,90.5,cm,
128	Node 92,91.5,cm,
129	Node 93,92.5,cm,
130	Node 94,93.5,cm,
131	~Inactive Nodes
132	0 line(s) of inactive nodes input follows.
133	~Rock or Soil Types
134	46 character(s) of rock or soil types notes follows.
135	Sand Properties from Touma and Vauclin (1986).
136	1 line(s) of rock or soil types input follows.
137	Sand,1,1,1,1,1,94,
138	~Mechanical Properties
139	1 line(s) of mechanical properties input follows.
140	Sand,0.370,0.312,0.2855,,,,constant,1.0,1.0,
141	~Hydraulic Properties
142	1 line(s) of hydraulic properties input follows.
143	Sand,4.2778e-3,4.2778e-3,4.2778e-3,hc:cm/s,,,,m^2,,1/m,
144	~Thermal Properties
145	0 line(s) of thermal properties input follows.
146	~Species Properties
147	0 line(s) of species properties input follows.
148	~Soil Characteristics
149	1 line(s) of soil characteristics input follows.
150	Sand,van Genuchten,0.044,1/cm,2.2,1.0E+20,m,,,,
151	~Liquid Relative Permeability Properties
152	1 line(s) of liquid relative permeability input follows.
153	Sand,Touma and Vauclin,1176.2012,6.07,1.0E-6,,
154	~Gas Relative Permeability Properties
155	1 line(s) of gas relative permeability input follows.
156	Sand,Touma and Vauclin,3.86e-5,-2.4,1.0e-20,
157	~Liquid Boundary Conditions
158	2 line(s) of liquid boundary conditions input follows.
159	Z-Direction: Top Surface,Dirichlet @ Boundary,101550.25,Pa (absolute),998.32, kg/m^3,0.0,1,1,1,1,94,94,
160	Z-Direction: Bottom Surface,Dirichlet @ Boundary,98778.685,Pa (absolute),998.32, kg/m^3,0.0,1,1,1,1,1,1,
161	~Gas Boundary Conditions
162	0 line(s) of gas boundary conditions input follows.
163	~Vapor Boundary Conditions
164	0 line(s) of vapor boundary conditions input follows.
165	~Energy Boundary Conditions
166	0 line(s) of energy boundary conditions input follows.
167	~Species Boundary Conditions
168	0 line(s) of species boundary conditions input follows.
169	~Initial Conditions
170	Gas Pressure & Liquid Pressure,
171	2 line(s) of initial conditions input follows.
172	Gas Pressure,101325.0,Pa (absolute),0.0,1/m,0.0,1/m,0.0,1/m,1,1,1,1,1,94,
173	Liquid Pressure,98778.685,Pa (absolute),0.0,1/cm,0.0,1/cm,-97.935192, 1/cm,1,1,1,1,1,94,
174	~Sources & Sinks
175	0 line(s) of sources & sinks input follows.
176	~Liquid Pathline Trace
177	0 line(s) of liquid pathline trace input follows.
178	~Output Control
179	1,1,1,1,1,94,zxplane,
180	8 line(s) of output control input follows.
181	0.05,h,
182	0.10,h,
183	0.15,h,
184	0.20,h,
185	0.25,h,
186	0.30,h,

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3 of 3

Exhibit 8.7. (Contd)

Line No.	Input File
127	Node 91,90.5,cm,
128	Node 92,91.5,cm,
129	Node 93,92.5,cm,
130	Node 94,93.5,cm,
131	~Inactive Nodes
132	0 line(s) of inactive nodes input follows.
133	~Rock or Soil Types
134	46 character(s) of rock or soil types notes follows.
135	Sand Properties from Touma and Vauclin (1986).
136	1 line(s) of rock or soil types input follows.
137	Sand,1,1,1,1,1,94,
138	~Mechanical Properties
139	1 line(s) of mechanical properties input follows.
140	Sand,0.370,0.312,0.2855,,,,constant,1.0,1.0,
141	~Hydraulic Properties
142	1 line(s) of hydraulic properties input follows.
143	Sand,4.2778e-3,4.2778e-3,4.2778e-3,hc:cm/s,,,,m^2,,1/m,
144	~Thermal Properties
145	0 line(s) of thermal properties input follows.
146	~Species Properties
147	0 line(s) of species properties input follows.
148	~Soil Characteristics
149	1 line(s) of soil characteristics input follows.
150	Sand,van Genuchten,0.044,1/cm,2.2,1.0E+20,m,,,,
151	~Liquid Relative Permeability Properties
152	1 line(s) of liquid relative permeability input follows.
153	Sand,Touma and Vauclin,1176.2012,6.07,1.0E-6,,
154	~Gas Relative Permeability Properties
155	1 line(s) of gas relative permeability input follows.
156	Sand,Touma and Vauclin,3.86e-5,-2.4,1.0e-20,
157	~Liquid Boundary Conditions
158	2 line(s) of liquid boundary conditions input follows.
159	Z-Direction: Top Surface,Dirichlet @ Boundary,101550.25,Pa (absolute),998.32, kg/m^3,0.0,1,1,1,1,94,94,
160	Z-Direction: Bottom Surface,Dirichlet @ Boundary,98778.685,Pa (absolute),998.32, kg/m^3,0.0,1,1,1,1,1,1,
161	~Gas Boundary Conditions
162	0 line(s) of gas boundary conditions input follows.
163	~Vapor Boundary Conditions
164	0 line(s) of vapor boundary conditions input follows.
165	~Energy Boundary Conditions
166	0 line(s) of energy boundary conditions input follows.
167	~Species Boundary Conditions
168	0 line(s) of species boundary conditions input follows.
169	~Initial Conditions
170	Gas Pressure & Liquid Pressure,
171	2 line(s) of initial conditions input follows.
172	Gas Pressure,101325.0,Pa (absolute),0.0,1/m,0.0,1/m,0.0,1/m,1,1,1,1,1,94,
173	Liquid Pressure,98778.685,Pa (absolute),0.0,1/cm,0.0,1/cm,-97.935192, 1/cm,1,1,1,1,1,94,
174	~Sources & Sinks
175	0 line(s) of sources & sinks input follows.
176	~Liquid Pathline Trace
177	0 line(s) of liquid pathline trace input follows.
178	~Output Control
179	1,1,1,1,1,94,zxplane,
180	8 line(s) of output control input follows.
181	0.05,h,
182	0.10,h,
183	0.15,h,
184	0.20,h,
185	0.25,h,
186	0.30,h,

Exhibit 8.7. (Contd)

Line No.	Input File
187	0.35,h,
188	0.40,h,
189	1,1,90,1,1,80,1,1,70,1,1,60,1,
190	0 line(s) of output control input follows.
191	4 line(s) of output control input follows.
192	Liquid Pressure,
193	Gas Pressure,
194	Liquid Saturation,
195	Volumetric Moisture Content,
196	4 line(s) of output control input follows.
197	Liquid Pressure,
198	Gas Pressure,
199	Liquid Saturation,
200	Liquid Phase Rel. Permeability,
201	~Surface Flux Integrator
202	0 line(s) of surface flux integrator input follows.
203	~Rock List
204	1 line(s) of rock list input follows.
205	Sand,
206	~

Exhibit 8.8. MSTS Input File for Two-Phase Infiltration Problem, Bounded Column

Line No. Input File

```
 1  ~Simulation Title and Notes
 2  beta,0001,
 3  1D Ponded Boundary Infiltration in Bounded Column
 4  W. E. Nichols
 5  Battelle, Pacific Northwest Laboratory
 6  Wednesday, October 7, 1992
 7  1:41:05 PM
 8  231 character(s) of simulation title notes follows.
 9  Simulation of infiltration in a bounded column after numerical and experimental
10  results reported in Touma and Vauclin (1986).  Initial conditions are computed f
11  rom the zero-hydraulic-gradient condition.  The Water-Air mode is used.
12  ~Solution Schemes
13  false,false,false,
14  banded matrix
15  false,true,true,false,
16  1.20,h,
17  0.0001,h,
18  1.5,
19  0.010,h,
20  true,false,true,true,true,false,
21  false,false,false,false,
22  ~Numerical Control
23  8,Maximum Residual,
24  1.0,h,1.0,h,
25  1.0E-06,1.0E-06,1.0E-06,
26  Geometric Mean,Geometric Mean,Geometric Mean,Geometric Mean,
27  ~Grid Geometry
28  cartesian
29  1,1,94,
30  1.0,cm,1.0,cm,94.0,cm,0.0,cm,-94.0,cm,
31  0.0,cm,
32  1 line(s) of grid geometry input follows.
33  Node 1,0.5,cm,
34  1 line(s) of grid geometry input follows.
35  Node 1,0.5,cm,
36  94 line(s) of grid geometry input follows.
37  Node 1,0.5,cm,
38  Node  2,1.5,cm,
39  Node  3,2.5,cm,
40  Node  4,3.5,cm,
41  Node  5,4.5,cm,
42  Node  6,5.5,cm,
43  Node  7,6.5,cm,
44  Node  8,7.5,cm,
45  Node  9,8.5,cm,
46  Node  10,9.5,cm,
47  Node  11,10.5,cm,
48  Node  12,11.5,cm,
49  Node  13,12.5,cm,
50  Node  14,13.5,cm,
51  Node  15,14.5,cm,
52  Node  16,15.5,cm,
53  Node  17,16.5,cm,
54  Node  18,17.5,cm,
55  Node  19,18.5,cm,
56  Node  20,19.5,cm,
57  Node  21,20.5,cm,
58  Node  22,21.5,cm,
59  Node  23,22.5,cm,
60  Node  24,23.5,cm,
61  Node  25,24.5,cm,
62  Node  26,25.5,cm,
63  Node  27,26.5,cm,
```

Exhibit 8.8. (Contd)

Line No.	Input File
64	Node 28,27.5,cm,
65	Node 29,28.5,cm,
66	Node 30,29.5,cm,
67	Node 31,30.5,cm,
68	Node 32,31.5,cm,
69	Node 33,32.5,cm,
70	Node 34,33.5,cm,
71	Node 35,34.5,cm,
72	Node 36,35.5,cm,
73	Node 37,36.5,cm,
74	Node 38,37.5,cm,
75	Node 39,38.5,cm,
76	Node 40,39.5,cm,
77	Node 41,40.5,cm,
78	Node 42,41.5,cm,
79	Node 43,42.5,cm,
80	Node 44,43.5,cm,
81	Node 45,44.5,cm,
82	Node 46,45.5,cm,
83	Node 47,46.5,cm,
84	Node 48,47.5,cm,
85	Node 49,48.5,cm,
86	Node 50,49.5,cm,
87	Node 51,50.5,cm,
88	Node 52,51.5,cm,
89	Node 53,52.5,cm,
90	Node 54,53.5,cm,
91	Node 55,54.5,cm,
92	Node 56,55.5,cm,
93	Node 57,56.5,cm,
94	Node 58,57.5,cm,
95	Node 59,58.5,cm,
96	Node 60,59.5,cm,
97	Node 61,60.5,cm,
98	Node 62,61.5,cm,
99	Node 63,62.5,cm,
100	Node 64,63.5,cm,
101	Node 65,64.5,cm,
102	Node 66,65.5,cm,
103	Node 67,66.5,cm,
104	Node 68,67.5,cm,
105	Node 69,68.5,cm,
106	Node 70,69.5,cm,
107	Node 71,70.5,cm,
108	Node 72,71.5,cm,
109	Node 73,72.5,cm,
110	Node 74,73.5,cm,
111	Node 75,74.5,cm,
112	Node 76,75.5,cm,
113	Node 77,76.5,cm,
114	Node 78,77.5,cm,
115	Node 79,78.5,cm,
116	Node 80,79.5,cm,
117	Node 81,80.5,cm,
118	Node 82,81.5,cm,
119	Node 83,82.5,cm,
120	Node 84,83.5,cm,
121	Node 85,84.5,cm,
122	Node 86,85.5,cm,
123	Node 87,86.5,cm,
124	Node 88,87.5,cm,
125	Node 89,88.5,cm,
126	Node 90,89.5,cm,

Exhibit 8.8. (Contd)

Line No.	Input File
127	Node 91,90.5,cm,
128	Node 92,91.5,cm,
129	Node 93,92.5,cm,
130	Node 94,93.5,cm,
131	~Inactive Nodes
132	0 line(s) of inactive nodes input follows.
133	~Rock or Soil Types
134	46 character(s) of rock or soil types notes follows.
135	Sand Properties from Touma and Vauclin (1986).
136	1 line(s) of rock or soil types input follows.
137	Sand,1,1,1,1,1,94,
138	~Mechanical Properties
139	1 line(s) of mechanical properties input follows.
140	Sand,0.370,0.312,0.2855,,,,constant,1.0,1.0,
141	~Hydraulic Properties
142	1 line(s) of hydraulic properties input follows.
143	Sand,4.2778e-3,4.2778e-3,4.2778e-3,hc:cm/s,,,,m^2,,1/m,
144	~Thermal Properties
145	0 line(s) of thermal properties input follows.
146	~Species Properties
147	0 line(s) of species properties input follows.
148	~Soil Characteristics
149	1 line(s) of soil characteristics input follows.
150	Sand,van Genuchten,0.044,1/cm,2.2,1.0E+20,m,,,,
151	~Liquid Relative Permeability Properties
152	1 line(s) of liquid relative permeability input follows.
153	Sand,Touma and Vauclin,1176.2012,6.07,1.0E-6,,
154	~Gas Relative Permeability Properties
155	1 line(s) of gas relative permeability input follows.
156	Sand,Touma and Vauclin,3.86e-5,-2.4,1.0e-20,
157	~Liquid Boundary Conditions
158	2 line(s) of liquid boundary conditions input follows.
159	Z-Direction: Top Surface,Dirichlet @ Boundary,101550.25,Pa (absolute),998.32, kg/m^3,0.0,1,1,1,1,94,94,
160	Z-Direction: Bottom Surface,Dirichlet @ Boundary,98778.685,Pa (absolute),998.32, kg/m^3,0.0,1,1,1,1,1,1,
161	~Gas Boundary Conditions
162	2 line(s) of gas boundary conditions input follows.
163	Z-Direction: Top Surface,Dirichlet @ Boundary,102921.3436,Pa (absolute),1.225, kg/m^3,0.0,1,1,1,1,94,94,
164	Z-Direction: Bottom Surface,Neumann @ Boundary,0.0,kg/m^2 s,,kg/m^3,0.0,1,1, 1,1,1,1,
165	~Vapor Boundary Conditions
166	0 line(s) of vapor boundary conditions input follows.
167	~Energy Boundary Conditions
168	0 line(s) of energy boundary conditions input follows.
169	~Species Boundary Conditions
170	0 line(s) of species boundary conditions input follows.
171	~Initial Conditions
172	Gas Pressure & Liquid Pressure,
173	2 line(s) of initial conditions input follows.
174	Gas Pressure,101325.0,Pa (absolute),0.0,1/m,0.0,1/m,0.0,1/m,1,1,1,1,1,94,
175	Liquid Pressure,98778.685,Pa (absolute),0.0,1/cm,0.0,1/cm,-97.935192,1/cm,1,1, 1,1,1,94,
176	~Sources & Sinks
177	0 line(s) of sources & sinks input follows.
178	~Liquid Pathline Trace
179	0 line(s) of liquid pathline trace input follows.
180	~Output Control
181	1,1,1,1,1,94,zxplane,
182	12 line(s) of output control input follows.
183	0.10,h,
184	0.20,h,

Exhibit 8.8. (Contd)

Line No.	Input File
185	0.30,h,
186	0.40,h,
187	0.50,h,
188	0.60,h,
189	0.70,h,
190	0.80,h,
191	0.90,h,
192	1.00,h,
193	1.10,h,
194	1.20,h,
195	1,1,90,1,1,80,1,1,70,1,1,60,1,
196	0 line(s) of output control input follows.
197	4 line(s) of output control input follows.
198	Liquid Pressure,
199	Gas Pressure,
200	Liquid Saturation,
201	Volumetric Moisture Content,
202	4 line(s) of output control input follows.
203	Liquid Pressure,
204	Gas Pressure,
205	Liquid Saturation,
206	Liquid Phase Rel. Permeability,
207	~Surface Flux Integrator
208	1 line(s) of surface flux integrator input follows.
209	Z-Direction: Top Surface,Gas Phase,1,1,1,1,94,94,
210	~Rock List
211	1 line(s) of rock list input follows.
212	Sand,
213	~

8.7 One-Dimensional Heat Pipe

The heat pipe problem involves a one-dimensional horizontal layer of porous medium subjected to a heat flux on one end and is characterized by high heat transfer rates and countercurrent flow of liquid and gas phases. Both phases are composed of water and air components (e.g., liquid water and dissolved air for the liquid phase, and air and water vapor for the gas phase). The specifics of the subject problem were described and solved by Udell and Fitch (1985) for constant physical properties at steady state. The Udell and Fitch model used a two-component gas phase made up of nitrogen and water vapor. A schematic of the problem proposed by Udell and Fitch is shown in Figure 8.11. The problem geometry consists of a tube, with an adiabatic wall, filled with a partially saturated porous medium. The right end of the tube is closed and subjected to a heat flux of 100 W/m^2. Conditions at the left end of the tube are maintained constant at total saturation, 70°C, and 101,330 Pa (absolute) gas pressure. Initial conditions within the tube are 0.7 liquid saturation, 70°C, and 101,330 Pa (absolute) gas pressure. The problem involves solving the transient response of the heat pipe from the initial conditions to steady-state conditions. The problem was selected to test the simulator's capability to model coupled two-phase flow, heat transport, and evaporation and condensation processes.

8.7.1 Problem Parameters and Input File

The soil-moisture-retention characteristics and saturation-relative-permeability functions for the porous media were described as shown in Equations (8.8) through (8.12). The Udell and Fitch model used a constant water-air surface tension value of 0.05878 N/m, instead of the

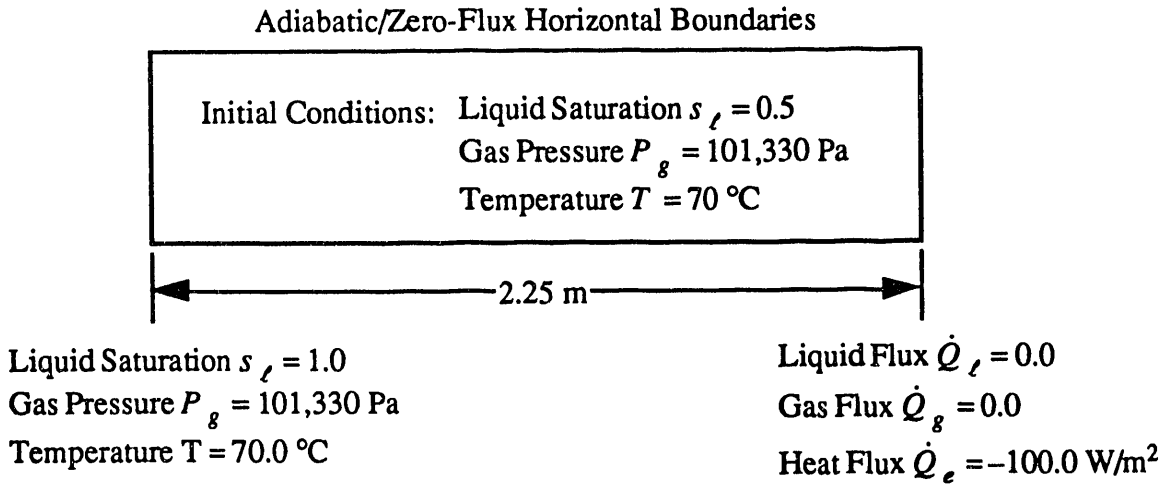

Figure 8.11. Schematic Describing the Heat Pipe Problem

temperature dependent model shown in Equation (8.9). The thermal conductivity of the porous medium was considered a function of the effective liquid saturation as shown in Equation (8.12). Properties for density, viscosity, heat of vaporization, and molecular diffusion coefficient were computed in MSTS as functions of local temperature and pressures; for the Udell and Fitch model, these parameters were considered constants. These constants, and other physical properties required to define the heat pipe problem, according to Udell and Fitch, are listed in Table 8.6. The input file for this problem is shown in Exhibit 8.9.

$$P_{cap} = P_g - P_\ell = \sigma^{aw} \left(\frac{n_D}{\tilde{k}} \right)^{\frac{1}{2}} \left[1.417 \left(1 - s_\ell^* \right) - 2.12 \left(1 - s_\ell^* \right)^2 + 1.263 \left(1 - s_\ell^* \right)^3 \right] \tag{8.8}$$

$$\sigma^{aw} = 0.2358 \left[1 - 0.625 \frac{(374.15 - T)}{647.3} \right] \left[\frac{(374.15 - T)}{647.3} \right]^{1.256} \tag{8.9}$$

$$k_{r\ell} = \left(s_\ell^* \right)^3 \tag{8.10}$$

$$k_{rg} = \left(1 - s_\ell^* \right)^3 \tag{8.11}$$

$$\tilde{k}_e = k_{dry} + \sqrt{s_\ell^*} \left(k_{wet} - k_{dry} \right) \tag{8.12}$$

where $k_{dry} = 0.582 \frac{\text{W}}{\text{m K}}$ and $k_{wet} = 1.130 \frac{\text{W}}{\text{m K}}$

Table 8.6. Heat Pipe Problem Physical Properties

Property Description	Symbol	Property Value
Dry-rock thermal conductivity	k_{dry}	0.582 W/m K
Wet-rock thermal conductivity	k_{wet}	1.130 W/m K
Gas density	ρ_g	0.960 kg/m^3
Liquid density	ρ_ℓ	958.4 kg/m^3
Gas kinematic viscosity	ν_g	21.0 x 10^{-6} m^2/s
Liquid kinematic viscosity	ν_ℓ	0.3066 x 10^{-6} m^2/s
Heat of vaporization	h_{vap}	2.257 x 10^6 J/kg
Intrinsic permeability	k	1.0 x 10^{-12} m^2
Surface tension	σ	0.05878 N/m
Molecular diffusion coefficient	D_g^{aw}	26.0 x 10^{-6} m^2/s
Nitrogen gas constant	R	461.52 J/kg mol K
Diffusive porosity	n_D	0.4
Gas tortuosity	τ_g	0.5
Heat flux	$\dot{Q}_e$	100.0 W/m^2

8.7.2 Simulation Results

The transient simulation begins by imbibing liquid water from the saturated boundary into the porous medium and increasing the temperature of the porous medium near the heat flux boundary. Liquid saturations near the heat flux boundary initially decrease because of the increased gas pressures. This initial decrease is followed by a short period of liquid saturation increase as the imbibed water from the saturated boundary reaches the other end of the pipe. The liquid saturations near the heat flux boundary then decrease to residual saturation levels as the temperature and pressures increase. The steady-state solution is characterized by three distinct regions within the heat pipe, as shown in Figures 8.12 through 8.14. Starting from the saturated boundary (left-hand side), the first region spans the distance from 0.0 to 0.5 m. This region is characterized by sharp gradients in temperature and air mole fractions as shown in Figures 8.12 and 8.13. Both

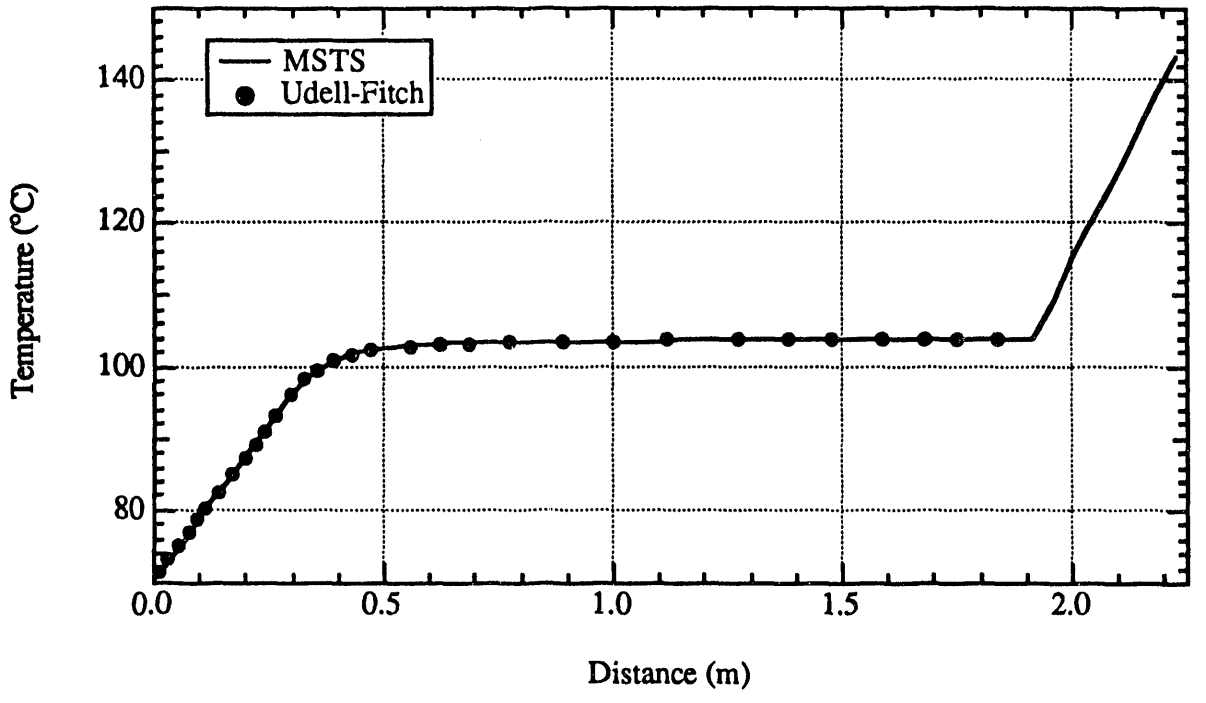

Figure 8.12. Steady-State Temperature Profiles for Heat Pipe Problem

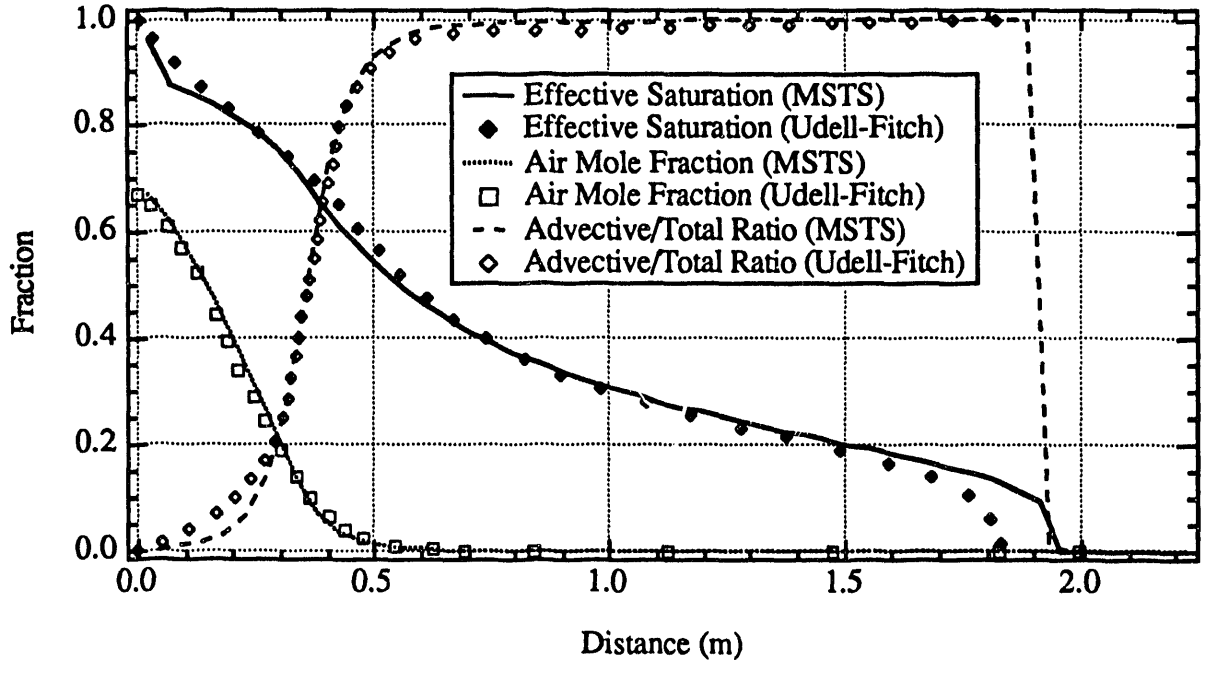

Figure 8.13. Steady-State Saturation, Air Mole Fraction, and Advective/Total Ratio Profiles for Heat Pipe Problem

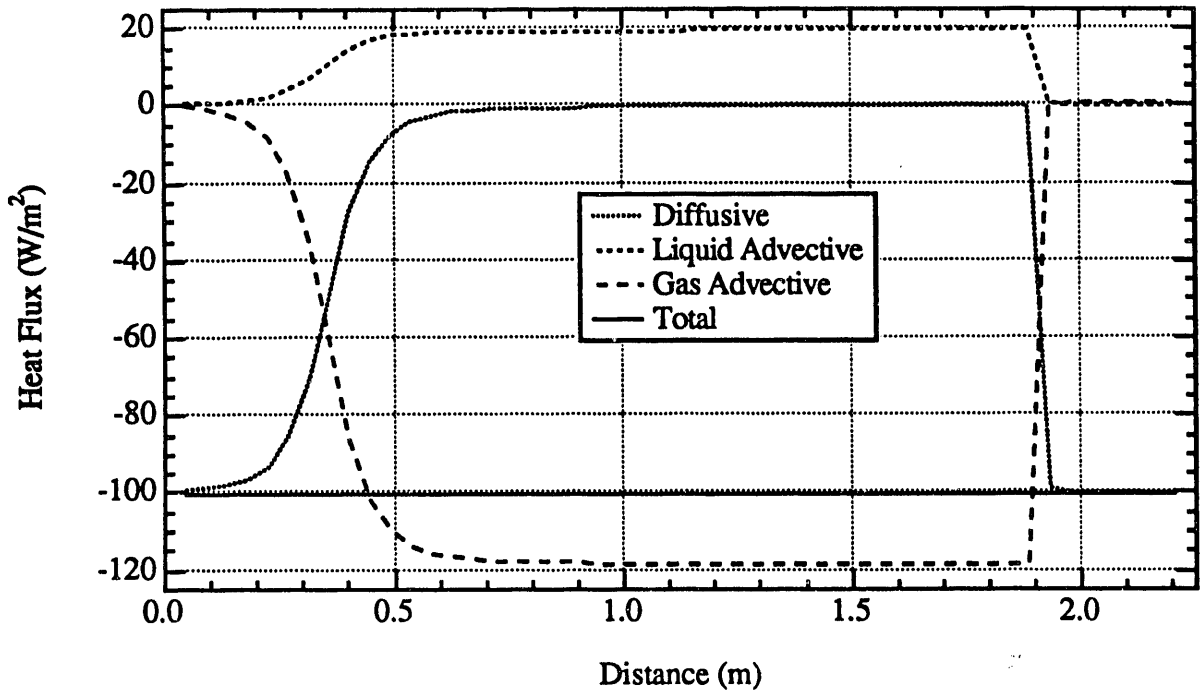

Figure 8.14. Steady-State Heat Transport Modes for Heat Pipe Problem

diffusive and advective heat transport mechanisms contribute to the overall heat transport. The second region spans from 0.5 m to 2.0 m, and is characterized by strong countercurrent gas- and liquid-phase flow and near-isothermal conditions. The gas phase flows toward the left end of the pipe and is composed primarily of pure water vapor. The liquid phase returns the condensed water to the desaturated region at the left end of the pipe. Heat transport in this region of the pipe is dominated by advection, as indicated by the near-isothermal conditions. The third region of the heat pipe spans from 2.0 m to 2.25 m, and is characterized by desaturated conditions. Heat transport in this region of the pipe is dominated by conduction. The MSTS results agree well with those computed by Udell and Fitch using a semi-analytical model with constant physical properties.

Exhibit 8.9. MSTS Input File for Heat Pipe Problem

Line No.	Input File
1	~Simulation Title and Notes
2	beta,0001,
3	Heat Pipe Problem
4	Mark White
5	Battelle, Pacific Northwest Laboratory
6	Wednesday, September 30, 1992
7	8:43:25 AM
8	199 character(s) of simulation title notes follows.
9	One-dimensional, horizontal, heat pipe problem. Liquid-gas countercurrent flow
10	with strong binary diffusion. Code verification against known analytical soluti
11	on (Udell and Fitch 1985; Pruess 1987).
12	~Solution Schemes
13	false,false,false,
14	banded matrix
15	true,true,true,false,
16	876.6,day,
17	0.005,day,
18	1.25,
19	100.0,day,
20	true,true,false,true,true,false,
21	false,false,false,false,
22	~Numerical Control
23	8,Maximum Residual,
24	1.0E+20,s,1.0E+20,s,
25	1.0E-06,1.0E-06,1.0E-06,
26	Harmonic Mean,Harmonic Mean,Harmonic Mean,Harmonic Mean,
27	~Grid Geometry
28	cartesian
29	50,1,1,
30	2.25,m,1.0,m,1.0,m,0.0,m,0.0,m,
31	0.0,m,
32	50 line(s) of grid geometry input follows.
33	Node 1,0.0225,m,
34	Node 2,0.0675,m,
35	Node 3,0.1125,m,
36	Node 4,0.1575,m,
37	Node 5,0.2025,m,
38	Node 6,0.2475,m,
39	Node 7,0.2925,m,
40	Node 8,0.3375,m,
41	Node 9,0.3825,m,
42	Node 10,0.4275,m,
43	Node 11,0.4725,m,
44	Node 12,0.5175,m,
45	Node 13,0.5625,m,
46	Node 14,0.6075,m,
47	Node 15,0.6525,m,
48	Node 16,0.6975,m,
49	Node 17,0.7425,m,
50	Node 18,0.7875,m,
51	Node 19,0.8325,m,
52	Node 20,0.8775,m,
53	Node 21,0.9225,m,
54	Node 22,0.9675,m,
55	Node 23,1.0125,m,
56	Node 24,1.0575,m,
57	Node 25,1.1025,m,
58	Node 26,1.1475,m,
59	Node 27,1.1925,m,
60	Node 28,1.2375,m,
61	Node 29,1.2825,m,
62	Node 30,1.3275,m,
63	Node 31,1.3725,m,

Exhibit 8.9. (Contd)

Line No.	Input File
64	Node 32,1.4175,m,
65	Node 33,1.4625,m,
66	Node 34,1.5075,m,
67	Node 35,1.5525,m,
68	Node 36,1.5975,m,
69	Node 37,1.6425,m,
70	Node 38,1.6875,m,
71	Node 39,1.7325,m,
72	Node 40,1.7775,m,
73	Node 41,1.8225,m,
74	Node 42,1.8675,m,
75	Node 43,1.9125,m,
76	Node 44,1.9575,m,
77	Node 45,2.0025,m,
78	Node 46,2.0475,m,
79	Node 47,2.0925,m,
80	Node 48,2.1375,m,
81	Node 49,2.1825,m,
82	Node 50,2.2275,m,
83	1 line(s) of grid geometry input follows.
84	Node 1,0.5,m,
85	1 line(s) of grid geometry input follows.
86	Node 1,0.5,m,
87	~Inactive Nodes
88	0 line(s) of inactive nodes input follows.
89	~Rock or Soil Types
90	0 character(s) of rock or soil types notes follows.
91	1 line(s) of rock or soil types input follows.
92	Porous Media,1,50,1,1,1,1,
93	~Mechanical Properties
94	1 line(s) of mechanical properties input follows.
95	Porous Media,0.4,0.4,0.34,,,,constant,,0.5,
96	~Hydraulic Properties
97	1 line(s) of hydraulic properties input follows.
98	Porous Media,1.0e-12,1.0e-12,1.0e-12,m^2,,,,m^2,,1/m,
99	~Thermal Properties
100	1 line(s) of thermal properties input follows.
101	Porous Media,somerton,0.582,0.582,0.582,1.13,1.13,1.13,W/m K,2600.0,kg/m^3,700.0, J/kg K,
102	~Species Properties
103	0 line(s) of species properties input follows.
104	~Soil Characteristics
105	1 line(s) of soil characteristics input follows.
106	Porous Media,Leverett,0.15,,632455.53,2.73582,m,,,,
107	~Liquid Relative Permeability Properties
108	1 line(s) of liquid relative permeability input follows.
109	Porous Media,Fatt and Klikoff,0.15,,1.e-6,,
110	~Gas Relative Permeability Properties
111	1 line(s) of gas relative permeability input follows.
112	Porous Media,Fatt and Klikoff,0.15,,1.e-6,
113	~Liquid Boundary Conditions
114	1 line(s) of liquid boundary conditions input follows.
115	X-Direction: West Surface,Dirichlet @ Boundary,101330.,Pa (absolute),998.32, kg/m^3,0.0,1,1,1,1,1,1,
116	~Gas Boundary Conditions
117	1 line(s) of gas boundary conditions input follows.
118	X-Direction: West Surface,Dirichlet @ Boundary,101330.,Pa (absolute),0.91944, kg/m^3,.21802,1,1,1,1,1,1,
119	~Vapor Boundary Conditions
120	1 line(s) of vapor boundary conditions input follows.
121	X-Direction: West Surface,Dirichlet @ Boundary,0.21802,1,1,1,1,1,1,
122	~Energy Boundary Conditions
123	2 line(s) of energy boundary conditions input follows.

Exhibit 8.9. (Contd)

Line No.	Input File
124	X-Direction: West Surface,Dirichlet @ Boundary,70,Celsius,2.864e+8,J/m^3, 5.2098e+5,J/m^3,1,1,1,1,1,1,
125	X-Direction: East Surface,Neumann @ Boundary,-100,W/m^2,,J/m^3,,J/m^3,50,50, 1,1,1,1,
126	~Species Boundary Conditions
127	0 line(s) of species boundary conditions input follows.
128	~Initial Conditions
129	Liquid Saturation & Gas Pressure,
130	3 line(s) of initial conditions input follows.
131	Gas Pressure,101330.0,Pa (absolute),0.0,1/m,0.0,1/m,0.0,1/m,1,50,1,1,1,1,
132	Liquid Saturation,0.5,,0.0,1/m,0.0,1/m,0.0,1/m,1,50,1,1,1,1,
133	Temperature,70.0,Celsius,0.0,1/m,0.0,1/m,0.0,1/m,1,50,1,1,1,1,
134	~Sources & Sinks
135	0 line(s) of sources & sinks input follows.
136	~Liquid Pathline Trace
137	0 line(s) of liquid pathline trace input follows.
138	~Output Control
139	1,50,1,1,1,1,xyplane,
140	0 line(s) of output control input follows.
141	35,1,1,40,1,1,45,1,1,50,1,1,1,
142	0 line(s) of output control input follows.
143	7 line(s) of output control input follows.
144	Liquid Pressure,
145	Gas Pressure,
146	Temperature,
147	Liquid Saturation,
148	Gas Phase Vapor Mass Fraction,
149	X-Dir. Liquid Velocity,
150	X-Dir. Gas Velocity,
151	7 line(s) of output control input follows.
152	Liquid Pressure,
153	Gas Pressure,
154	Temperature,
155	Liquid Saturation,
156	Gas Phase Vapor Mass Fraction,
157	X-Dir. Liquid Velocity,
158	X-Dir. Gas Velocity,
159	~Surface Flux Integrator
160	0 line(s) of surface flux integrator input follows.
161	~Rock List
162	1 line(s) of rock list input follows.
163	Porous Media,
164	~

8.8 Unsaturated Transport

This problem considers transport in a one-dimensional, semi-infinite, horizontal tube of partially saturated soil. The object is to determine the concentration field in a tube of soil that has a uniform initial concentration and moisture content and in which the upstream boundary is subject to a prescribed moisture content and solute concentration. Transport processes include both advection and hydrodynamic dispersion, with both the hydraulic diffusivity and the hydraulic dispersion being functions of moisture content. This problem was proposed by Ross et al. (1982) as a test problem, and results are compared with those obtained from a semi-analytical solution reported by Smiles et al. (1977). The water transport problem on which this transport case is imposed is the horizontal infiltration problem for which Philip (1955) provided a semi-analytical solution.

8.8.1 Problem Domain and Input Parameters

This problem considers transport in an unsaturated flow field calculated for a one-dimensional, horizontal pipe. The objective is to determine the species concentration field in a tube of soil with porosity 0.45, a uniform initial species concentration and moisture content, and an upstream boundary that is maintained at a prescribed moisture content and a prescribed solute concentration. Transport processes includes both advection and hydrodynamic dispersion, with both hydraulic diffusivity and hydraulic dispersion as functions of moisture content ($D_s(\theta) = \theta D$, where D is equal to 1.0 cm^2/day in this problem).

The liquid-phase boundary conditions are saturation commencing at time zero on the west (left, or $x = 0$ cm) boundary and a constant saturation of 0.444 (initial condition) at the east (right, or $x = 20$ cm) boundary. The species boundary conditions are 1.0 g/L concentration commencing at time zero at the west boundary and 0.1 g/L at the east boundary. MSTS species concentrations are always indicated in terms of moles or curies per volume, but mass per volume (g/L in this case) may also be used so long as this usage is consistent. Note that concentrations at boundaries are expressed with respect to the volume of the phase (i.e., 1.0 g/L of water at the west boundary) while concentrations for initial conditions are expressed with respect to total volume. The initial conditions are: gas pressure, 101,325 Pa (absolute); liquid saturation, 0.444; species concentration, 0.1 g/L; and temperature, 20.0°C. The species concentration proposed by Ross et al. (1982) (0.1 g/L) is in terms of water volume, so we must express this value in terms of total volume for MSTS. Multiplying 0.1 g/L by the moisture content (which is the ratio of water volume to total volume), we obtain 0.1 g/L_{wtr} x 0.2 L_{wtr}/L_{tot} = 0.02 g/L_{tot}.

8.8.2 Semi-Analytic Solution

Philip (1955) introduced a semi-analytical solution to the one-dimensional flow domain represented in this unsaturated transport problem. Smiles et al. (1977) reported the semi-analytical solution for the transport.

8.8.3 Numerical Accuracy

The spatial and temporal discretization requires careful attention so that stability is ensured in solving the dilute species mass conservation equation. A discretization or time stepping that is too large may result in excessive numerical dispersion, which would result in unacceptable error in predictions of solute transport. We base the maximum grid size for the domain in which dilute species transport is to be modeled on the criterion (Huyakorn and Pinder 1983; Price et al. 1966)

$$Pe = \frac{u\,\Delta x}{\tau_\ell\, s_\ell\, n_D\, D} \leq 2 \tag{8.13}$$

where Pe = Peclet Number

u = Darcy velocity in x-direction, cm/day

Δx = grid cell length in x-direction, cm

τ_ℓ = liquid-phase tortuosity

s_ℓ = liquid saturation

n_D = diffusive porosity

D = molecular diffusivity, cm^2/day.

The expression in Equation (8.13) reflects the one-dimensional nature of this problem (i.e., we are not concerned with the Peclet Number in other dimensions). The liquid-phase tortuosity in this problem is 1, the diffusive porosity is 0.45, and the molecular diffusivity is 1.0 cm^2/day. To determine the maximum permissible Δx requires values for the Darcy velocity in the x-direction and the liquid saturation, both of which are time-varying in this problem. By performing preliminary simulations with MSTS for the water conservation equation only, we find that early peak velocities are on the order of 22.3 cm/day, and the associated volumetric moisture content (equal to the product $s_\ell n_D$) is 0.445. Substituting these values into Equation (8.13), we obtain

$$\Delta x \leq \frac{2\,\tau_\ell\, s_\ell\, n_D\, D}{u} = \frac{2\,(1.0)\,(0.445)\,(1.0\ \text{cm}^2/\text{day})}{22.3\ \text{cm/day}} = 0.0399\ \text{cm} \approx 0.04\ \text{cm}$$

The maximum permissible time step is similarly determined by following the criterion

$$Cr = \frac{u\,\Delta t}{\Delta x} \leq 1 \tag{8.14}$$

where Cr is the Courant Number. This is merely a mathematical expression for the criterion that the time required for fluid to transit the grid cell length must be less than the time-step duration. Again, substituting:

$$\Delta t \leq \frac{\Delta x}{u} = \frac{0.04\ \text{cm}}{22.3\ \text{cm/day}} = 0.00179\ \text{day} \approx 150\ \text{seconds}$$

Therefore, the input file shown in Exhibit 8.10 uses a grid cell length of 0.04 cm for the portion of the domain between 0.0 and 4.5 cm (Exhibit 8.10, Grid Geometry card, lines 31-190). Somewhat larger grid cells are used beyond 4.5 cm because that is the maximum distance we expect the solute front to reach in the 0.11 day; hence, the 0.04-cm resolution is not required beyond 4.5 cm. The maximum time step is restricted to 150 seconds (Exhibit 8.10, Solution Schemes card, line 23). A final caution: nothing in the MSTS code will prevent the user from exceeding the Peclet or Courant limits discussed here. It is the responsibility of the modeler to ensure numerical accuracy through appropriate spatial- and temporal-discretization choices.

8.8.4 Simulation Results and Comparison to Semi-Analytic Solution

The total time simulated for this problem was 9504 seconds (0.11 day). The "dimensionless concentrations" at 0.01, 0.06, and 0.11 day reported in Ross et al. (1982) for the Smiles et al. (1977) semi-analytical solution are shown as solid lines in Figure 8.15. The MSTS solution for the input file shown in Exhibit 8.10 is shown as one dashed line (labeled "$\Delta x = 0.04$ cm" in the legend), while a second MSTS solution using a grid spacing of only 0.02 cm and a maximum time step of 75 seconds is shown as a second dashed line ("$\Delta x = 0.02$ cm" in the legend). Note that decreasing the grid spacing (and hence the time spacing) to meet the Courant limit reduces the numerical dispersion for this strongly advection-driven problem. Further reductions in the time and space stepping would bring even better predictions compared to the semi-analytical solution, but at the price of greater computer time requirements to solve the problem.

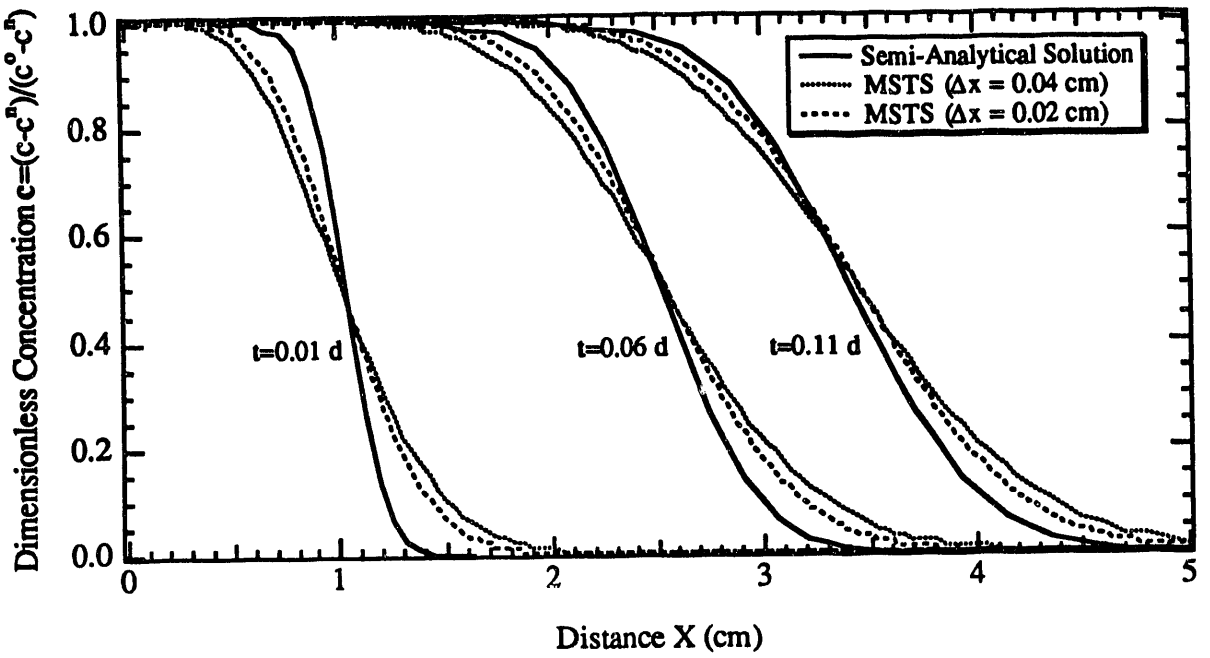

Figure 8.15. Dimensionless Solute Concentration Versus Distance at Various Times Using the Semi-Analytical Solution of Smiles et al. (1977) and MSTS Solutions With Two Spatial and Temporal Discretizations

The dimensionless concentration was not a direct output of MSTS, but was computed using MSTS output. MSTS reports species concentration in units of mol/L, where the volumetric measure (liters) refers to total volume (not water volume, as Smiles et al. [1977] reports it). Therefore, we divide each concentration reported by MSTS by the corresponding moisture content for the time and cell to obtain the concentration with respect to the aqueous phase. This value is converted into a dimensionless concentration by scaling it between the values at each boundary so that all concentrations have a value between 0 (initial condition) and 1 (maximum concentration).

Exhibit 8.10. MSTS Input File for Unsaturated Transport Problem

Line No.	Input File
1	~Simulation Title and Notes
2	beta,0001,
3	Specie Transport
4	W.E. Nichols
5	Battelle, Pacific Northwest Laboratory
6	Friday, September 18, 1992
7	2:48:00 PM
8	505 character(s) of simulation title notes follows.
9	This problem considers transport in the flow field calculated for a horizontal u
10	nsaturated pipe. The object is to determine the specie concentration field in a
11	tube of soil that has a uniform initial specie concentration and moisture conte
12	nt, with an upstream boundary that has a prescribed moisture content and solute
13	concentration. Transport processes include both advection and hydrodynamic disp
14	ersion, with both the hydraulic diffusivity and hydraulic dispersion being funct
15	ions of moisture content.
16	~Solution Schemes
17	false,false,false,
18	banded matrix
19	false,true,false,true,
20	9504.0,s,
21	1.0,s,
22	1.5,
23	150.0,s,
24	true,false,true,true,false,false,
25	false,false,false,false,
26	~Numerical Control
27	8,Maximum Residual,
28	1.0,h,1.0,h,
29	1.0e-6,1.0e-6,1.0e-6,
30	Harmonic Mean,Harmonic Mean,Harmonic Mean,Harmonic Mean,
31	~Grid Geometry
32	cartesian
33	150,1,1,
34	20.0,cm,1,m,1,m,0.0,m,0.0,m,
35	0.0,m,
36	150 line(s) of grid geometry input follows.
37	Node 1,0.02,cm,
38	Node 2,0.06,cm,
39	Node 3,0.1,cm,
40	Node 4,0.14,cm,
41	Node 5,0.18,cm,
42	Node 6,0.22,cm,
43	Node 7,0.26,cm,
44	Node 8,0.3,cm,
45	Node 9,0.34,cm,
46	Node 10,0.38,cm,
47	Node 11,0.42,cm,
48	Node 12,0.46,cm,
49	Node 13,0.5,cm,
50	Node 14,0.54,cm,
51	Node 15,0.58,cm,
52	Node 16,0.62,cm,
53	Node 17,0.66,cm,
54	Node 18,0.7,cm,
55	Node 19,0.74,cm,
56	Node 20,0.78,cm,
57	Node 21,0.82,cm,
58	Node 22,0.86,cm,
59	Node 23,0.9,cm,
60	Node 24,0.94,cm,
61	Node 25,0.98,cm,
62	Node 26,1.02,cm,
63	Node 27,1.06,cm,

Exhibit 8.10. (Contd)

Line No.	Input File
64	Node 28,1.1,cm,
65	Node 29,1.14,cm,
66	Node 30,1.18,cm,
67	Node 31,1.22,cm,
68	Node 32,1.26,cm,
69	Node 33,1.3,cm,
70	Node 34,1.34,cm,
71	Node 35,1.38,cm,
72	Node 36,1.42,cm,
73	Node 37,1.46,cm,
74	Node 38,1.5,cm,
75	Node 39,1.54,cm,
76	Node 40,1.58,cm,
77	Node 41,1.62,cm,
78	Node 42,1.66,cm,
79	Node 43,1.7,cm,
80	Node 44,1.74,cm,
81	Node 45,1.78,cm,
82	Node 46,1.82,cm,
83	Node 47,1.86,cm,
84	Node 48,1.9,cm,
85	Node 49,1.94,cm,
86	Node 50,1.98,cm,
87	Node 51,2.02,cm,
88	Node 52,2.06,cm,
89	Node 53,2.1,cm,
90	Node 54,2.14,cm,
91	Node 55,2.18,cm,
92	Node 56,2.22,cm,
93	Node 57,2.26,cm,
94	Node 58,2.3,cm,
95	Node 59,2.34,cm,
96	Node 60,2.38,cm,
97	Node 61,2.42,cm,
98	Node 62,2.46,cm,
99	Node 63,2.5,cm,
100	Node 64,2.54,cm,
101	Node 65,2.58,cm,
102	Node 66,2.62,cm,
103	Node 67,2.66,cm,
104	Node 68,2.7,cm,
105	Node 69,2.74,cm,
106	Node 70,2.78,cm,
107	Node 71,2.82,cm,
108	Node 72,2.86,cm,
109	Node 73,2.9,cm,
110	Node 74,2.94,cm,
111	Node 75,2.98,cm,
112	Node 76,3.02,cm,
113	Node 77,3.06,cm,
114	Node 78,3.1,cm,
115	Node 79,3.14,cm,
116	Node 80,3.18,cm,
117	Node 81,3.22,cm,
118	Node 82,3.26,cm,
119	Node 83,3.3,cm,
120	Node 84,3.34,cm,
121	Node 85,3.38,cm,
122	Node 86,3.42,cm,
123	Node 87,3.46,cm,
124	Node 88,3.5,cm,
125	Node 89,3.54,cm,
126	Node 90,3.58,cm,

Exhibit 8.10. (Contd)

Line No.	Input File
127	Node 91,3.62,cm,
128	Node 92,3.66,cm,
129	Node 93,3.7,cm,
130	Node 94,3.74,cm,
131	Node 95,3.78,cm,
132	Node 96,3.82,cm,
133	Node 97,3.86,cm,
134	Node 98,3.9,cm,
135	Node 99,3.94,cm,
136	Node 100,3.98,cm,
137	Node 101,4.02,cm,
138	Node 102,4.06,cm,
139	Node 103,4.1,cm,
140	Node 104,4.14,cm,
141	Node 105,4.18,cm,
142	Node 106,4.22,cm,
143	Node 107,4.26,cm,
144	Node 108,4.3,cm,
145	Node 109,4.34,cm,
146	Node 110,4.38,cm,
147	Node 111,4.42,cm,
148	Node 112,4.46,cm,
149	Node 113,4.5,cm,
150	Node 114,4.6,cm,
151	Node 115,4.7,cm,
152	Node 116,4.8,cm,
153	Node 117,4.9,cm,
154	Node 118,5,cm,
155	Node 119,5.1,cm,
156	Node 120,5.2,cm,
157	Node 121,5.3,cm,
158	Node 122,5.4,cm,
159	Node 123,5.5,cm,
160	Node 124,5.6,cm,
161	Node 125,5.7,cm,
162	Node 126,5.8,cm,
163	Node 127,5.9,cm,
164	Node 128,6,cm,
165	Node 129,6.2,cm,
166	Node 130,6.4,cm,
167	Node 131,6.6,cm,
168	Node 132,6.8,cm,
169	Node 133,7,cm,
170	Node 134,7.2,cm,
171	Node 135,7.4,cm,
172	Node 136,7.6,cm,
173	Node 137,7.8,cm,
174	Node 138,8,cm,
175	Node 139,8.5,cm,
176	Node 140,9.5,cm,
177	Node 141,10.5,cm,
178	Node 142,11.5,cm,
179	Node 143,12.5,cm,
180	Node 144,13.5,cm,
181	Node 145,14.5,cm,
182	Node 146,15.5,cm,
183	Node 147,16.5,cm,
184	Node 148,17.5,cm,
185	Node 149,18.5,cm,
186	Node 150,19.5,cm,
187	1 line(s) of grid geometry input follows.
188	Node 1,0.5,m,
189	1 line(s) of grid geometry input follows.

Exhibit 8.10. (Contd)

Line No.	Input File
190	Node 1,0.5,m,
191	~Inactive Nodes
192	0 line(s) of inactive nodes input follows.
193	~Rock or Soil Types
194	0 character(s) of rock or soil types notes follows.
195	1 line(s) of rock or soil types input follows.
196	Generic Sand,1,150,1,1,1,1,
197	~Mechanical Properties
198	1 line(s) of mechanical properties input follows.
199	Generic Sand,0.45,0.45,0.30,,,,constant,1.0,0.0,
200	~Hydraulic Properties
201	1 line(s) of hydraulic properties input follows.
202	Generic Sand,1.0,1.0,1.0,hc:cm/day,,,,hc:cm/day,0.0,1/m,
203	~Thermal Properties
204	0 line(s) of thermal properties input follows.
205	~Species Properties
206	1 line(s) of species properties input follows.
207	Generic Sand,Generic Solute,1.1574074E-9,m^2/s,1.1574074E-9,m^2/s,1.0e+20, cm^3 gas/gm liq.,0.0,gm liq./gm sol.,,s,
208	~Soil Characteristics
209	1 line(s) of soil characteristics input follows.
210	Generic Sand,Tabular,Table No. 1,
211	2 line(s) of capillary tables input follows.
212	1.0,.333333,m,
213	0.0,1.0,m,
214	~Liquid Relative Permeability Properties
215	1 line(s) of liquid relative permeability input follows.
216	Generic Sand,Tabular vs Liquid Saturation,Table No. 1,
217	2 line(s) of liquid permeability tables input follows.
218	0.33333,0.0,
219	1.0,1.0,
220	~Gas Relative Permeability Properties
221	0 line(s) of gas relative permeability input follows.
222	~Liquid Boundary Conditions
223	1 line(s) of liquid boundary conditions input follows.
224	X-Direction: West Surface,Dirichlet @ Boundary,101325.0,Pa (absolute),998.31, kg/m^3,0.0,1,1,1,1,1,1,
225	~Gas Boundary Conditions
226	0 line(s) of gas boundary conditions input follows.
227	~Vapor Boundary Conditions
228	0 line(s) of vapor boundary conditions input follows.
229	~Energy Boundary Conditions
230	0 line(s) of energy boundary conditions input follows.
231	~Species Boundary Conditions
232	2 line(s) of species boundary conditions input follows.
233	X-Direction: West Surface,Dirichlet @ Boundary,1.0,(mol;ci)/liter,,,1,1,1,1,1,1,
234	X-Direction: East Surface,Dirichlet @ Boundary,0.1,(mol;ci)/liter,,,150,150, 1,1,1,1,
235	~Initial Conditions
236	Liquid Saturation & Gas Pressure,
237	3 line(s) of initial conditions input follows.
238	Gas Pressure,101325.0,Pa (absolute),0.0,1/m,0.0,1/m,0.0,1/m,1,150,1,1,1,1,
239	Liquid Saturation,0.4444,,0.0,1/m,0.0,1/m,0.0,1/m,1,150,1,1,1,1,
240	Species Concentration,0.02,(mol;ci)/liter,0.0,1/m,0.0,1/m,0.0,1/m,1,150,1,1,1,1,
241	~Sources & Sinks
242	0 line(s) of sources & sinks input follows.
243	~Liquid Pathline Trace
244	0 line(s) of liquid pathline trace input follows.
245	~Output Control
246	1,150,1,1,1,1,xyplane,
247	3 line(s) of output control input follows.
248	0.01,day,
249	0.06,day,

Exhibit 8.10. (Contd)

Line No.	Input File
250	0.11,day,
251	5,1,1,10,1,1,15,1,1,20,1,1,1,
252	0 line(s) of output control input follows.
253	2 line(s) of output control input follows.
254	Species Concentration,
255	Volumetric Moisture Content,
256	4 line(s) of output control input follows.
257	Liquid Pressure,
258	Species Concentration,
259	Volumetric Moisture Content,
260	X-Dir. Liquid Velocity,
261	~Surface Flux Integrator
262	0 line(s) of surface flux integrator input follows.
263	~Rock List
264	1 line(s) of rock list input follows.
265	Generic Sand,
266	~

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