SAMFT1D 2_0

SAMFT1D
Single-phase And Multiphase Flow and Transport in 1 Dimension

Version 2.0

DOCUMENTATION AND USER'S GUIDE

Prepared by
Y.S. Wu
P.S. Huyakorn
S. Panday
N.S. Park
J.B. Kool
HydroGeoLogic, Inc.
Herndon, VA 22070

Prepared for
Los Alamos National Laboratory
Los Alamos, NM 87545

September, 1991

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ABSTRACT

This report documents a one-dimensional numerical model, SAMFT1D, developed to simulate single-phase and multiphase fluid flow and solute transport in variably saturated porous media. The formulation of the governing equations and the numerical procedures used in the code for single-phase and multiphase flow and transport are presented. The code is constructed to handle single-phase as well as two- or three-phase flow conditions using two integrated sets of computational modules. The fully implicit scheme is used in the code for both single-phase and multiphase flow simulations. Either the Crank-Nicholson scheme or the fully implicit scheme may be used in the transport simulation. The single-phase modules employ the Galerkin and upstream weighted residual finite element techniques to model flow and transport of water (aqueous phase) containing dissolved single-species contaminants concurrently or sequentially, and include the treatment of various boundary conditions and physical processes. The multiphase flow modules use block-centered finite difference techniques to simulate two- or three-phase flow problems, and treat different boundary conditions in terms of source/sink terms fully implicitly. Whereas the multiphase solute transport modules employ finite element schemes to handle single-species transport in multiphase fluid systems. Several benchmark problems are presented to verify the code and to demonstrate its utility. These sample problems range from one-phase unsaturated flow and transport to two- and three-phase flow problems including gravity and capillary effects and associated transport simulations.

This document has been produced as a user's manual. It contains detailed information on the code structure along with instructions for input data preparation and sample input and

printed output for selected test problems. Also included are instructions for job set up and simulation restart procedures.

ACKNOWLEDGEMENTS

The authors gratefully acknowledge Dr. Peter A. Forsyth (Dept. of Computer Science, University of Waterloo, Waterloo, Ontario, Canada) for his guidance and contribution in the development and verification of the SAMFT1D code. Thanks are also due to Dr. Edward A. Sudicky of the University of Waterloo for advice on designing the test problems.

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1 INTRODUCTION

1.1 BACKGROUND AND PURPOSE OF THE CODE

SAMFT1D is a one-dimensional numerical code that simulates fluid flow and solute transport in variably saturated porous media. The code is intended to handle single-phase as well as two-phase and three-phase flow conditions using two integrated sets of computational modules. The single-phase flow and transport computational modules employ finite element techniques to simulate situations involving flow of water (aqueous phase) and single-species transport of dissolved contaminants. Efficient matrix computational and solution schemes are employed in conjunction with simple linear one-dimensional elements to analyze problems involving highly nonlinear soil moisture characteristics.

The multiphase flow modules are coded using fully-implicit block-centered finite difference techniques to simulate two-phase (water and NAPL - Non Aqueous Phase Liquid) flow in a two-phase system, or two-phase flow (water and NAPL, in a three-phase (water, NAPL and air) system, or three-phase flow problems. The multiphase solute transport modules use the finite element scheme to simulate a single-species contaminant component transport in porous media including the maximum solubility constraint for the component. Several commonly encountered boundary conditions for groundwater and soil contamination near surface, such as prescribed pressure or flux, water table, recharge or infiltration conditions are incorporated in the code. Both fluid flow and solute transport simulations in SAMFT1D can be handled concurrently or sequentially.

1.2 OVERVIEW OF CODE CAPABILITIES AND SALIENT FEATURES

Modeling of fluid flow and waste migration in variably saturated subsurface systems can be a formidable task unless one is equipped with a proper code that accommodates various conditions. Recognizing this point, SAMFT1D was developed to have not only essential modeling capabilities but also salient features that facilitate practical use. An overview of these aspects of the code is presented below.

1. SAMFT1D can perform transient analyses or (whenever practical) single step steady-state analyses of both variably saturated water flow and solute transport problems. An option to include hysteresis in the transient single-phase flow simulation is also available. In a multiphase flow simulation, tabular or functional form of constitutive relations may be used. If the flow and transport problems are associated, a dual simulation can be made by solving the problems concurrently or sequentially in a single computer run.

2. The numerical formulations and nonlinear solution procedures in SAMFT1D are based on the state-of-the-art technology designed to accommodate a wide range of flow conditions (one, two and three active phases) including highly nonlinear fluid retention characteristics, material heterogeneity (layering), and rapidly fluctuating transient flow boundary conditions.

3. The flow simulator of SAMFT1D can handle various boundary conditions and physical processes including transient infiltration, and water table conditions. Temporal variations of pressure and flux boundary conditions can be handled conveniently using either continuous piecewise linear representations or discontinuous (stepped) representations.

4. The transport simulator of SAMFT1D is designed to have upstream weighting capability to circumvent numerical oscillations. The scheme can accommodate first-order decay as well as linear retardation. Both pulse and step releases of contaminants can be simulated. Additionally, the solubility limit of the modeled contaminant can be incorporated in the transport simulation and mass balance calculation. These capabilities make it advantageous to use SAMFT1D in the prediction of fate and transport of miscible and immiscible contaminants with dissolved constituents.

1.3 APPLICABILITY OF THE CODE

The SAMFT1D has many practical applications. Typical examples include the following:

- Investigation of multiphase immiscible flow involving NonAqueous Phase Liquids (NAPL) and miscible transport of dissolved constituents or components in the unsaturated zone of the subsurface system
- Investigation of moisture movement in variably saturated soil and subsurface systems
- Investigation of transport of dissolved contaminants in the subsurface soil system
- Investigation of potential for radionuclide migration from subsurface repositories or buried waste containers.

1.4 CODE USER REQUIREMENTS

In order to apply the SAMFT1D code effectively, the user will need:

- a thorough understanding of hydrogeological principles
- a basic understanding of finite element and finite difference techniques
- an awareness of the code's capabilities and limitations

- familiarity with the editor, operating system, and file handling concepts of the computer system used.

It is also recommended that the user run some of the test problems provided to gain confidence and understanding in using the code.

1.5 COMPUTER EQUIPMENT REQUIREMENTS

SAMFT1D is written in ANSI Standard FORTRAN 77 and can be compiled on any standard micro, mini, or mainframe system. The source code was developed and tested on the MIPS work station and a PC 386 machine using the FORTRAN 77 compiler developed by the University of Salford, United Kingdom. Installation of earlier versions of the code has also been made on VAX, micro-VAX, MIPS and SUN computers with standard FORTRAN 77 compilers. With minor conversion (e.g., changing OPEN FILE statements), the source code can be made to compile and run on any PC 386 machine properly equipped with at least 2 megabytes of core memory, a protected mode FORTRAN 77 compiler, and a 80387 or Weitek math co-processor.

2 GOVERNING MATHEMATICAL MODELS

2.1 PROCESS AND GEOMETRY

The single-phase computational modules of SAMFT1D perform one-dimensional simulations of water flow and/or solute transport in variably saturated or fully saturated porous media. These modules employ the state-of-the-art finite element technology to provide efficient steady-state and transient solutions of practical problems encountered in the investigation, mitigation and remediation of soil and groundwater contamination due to disposal of chemical and/or nuclear wastes. The steady-state analysis is performed by disregarding all storage terms of the governing equations thus avoiding the necessity of time marching. The transient analysis is performed by time marching until the prescribed number of time steps is reached. For water flow simulations, the code can handle a variety of boundary conditions including infiltration, evaporation, and sinks and sources of water and solute. The code can also accommodate severely nonlinear soil moisture characteristics and layering of permeability. For solute transport simulations, SAMFT1D accounts for advection, hydrodynamic dispersion, equilibrium sorption, and first-order decay.

The multiphase flow modules of SAMFT1D perform one-dimensional (block-centered) finite difference simulations of two-phase or three-phase fluid flow in porous media. The fluids considered include water, NAPL (NonAqueous Phase Liquid) contaminant, and air. The multiphase solute transport modules of SAMFT1D employ the finite element method to perform analyses of single component contamination problems in multiphase soil or groundwater systems.

In performing the analysis of a single-phase or multiphase flow problem, the user is permitted to employ the following coordinate system:

- one-dimensional x-coordinate along a horizontal direction
- one-dimensional z-coordinate along a downward vertical direction.

2.2 GOVERNING AND SUPPLEMENTARY EQUATIONS FOR SINGLE-PHASE MODELS

The single-phase components of SAMFT1D are formulated based upon two governing equations, one describing flow of water (aqueous-phase) and the other describing single-component solute transport. Both equations are described in this section together with initial and boundary conditions as well as other relevant supplementary constitutive relations.

2.2.1 Variably Saturated Flow

For single-phase, variably saturated flow analysis, the SAMFT1D code uses gauge pressure head of water (the aqueous phase) as the primary dependent variable. The governing equation for one-dimensional flow in a vertical direction is given by:

$$\frac{\partial}{\partial z}\left[K k_{rw} \left(\frac{\partial \psi}{\partial z} - 1 \right) \right] = \eta \frac{\partial \psi}{\partial t} \qquad (2.1)$$

where ψ is the gauge, water-pressure head, K is the saturated hydraulic conductivity, k_{rw} is the relative permeability to water, z is the downward vertical coordinate, t is time, and η is an effective water storage capacity, defined as

$$\eta = S_w S_s + \phi \frac{dS_w}{d\psi} \tag{2.2}$$

where S_s is specific storage, S_w is water saturation, and ϕ is the effective porosity. Note that ψ and K are defined as

$$\psi = (P_w - P_{atm})/\rho_w g \tag{2.3}$$

and

$$K = k\rho_w g/\mu_w \tag{2.4}$$

where P_w is the water-phase pressure, P_{atm} is the atmospheric pressure, ρ_w is the water density, g is the gravitational acceleration constant, k is the intrinsic permeability, and μ_w is the dynamic viscosity of water.

The initial and boundary conditions are given by

$$\psi(z,0) = \psi_i \tag{2.5}$$

and

$$\psi(z_B,t) = \tilde{\psi} \tag{2.6a}$$

or

$$V(z_B,t) = I \tag{2.6b}$$

where ψ_i is the initial pressure head value, z_B is the coordinate of a boundary node

(z_B=0 or z_B=L, where L is the length of the soil column), $\tilde{\psi}$ is the prescribed head value, and I is the flux distribution or infiltration rate.

The formulation presented is for a one-dimensional vertical flow problem. It can be readily adapted to a simpler situation of one-dimension horizontal flow.

To solve the variably saturated infiltration problem, it is also necessary to specify the relationships of relative permeability versus water saturation and pressure head versus water saturation. Two alternative function expressions are used to describe the relationship of relative permeability versus water saturation. These functions are given by (Brook and Corey, 1966; van Genuchten, 1980):

$$k_{rw} = S_e^n \tag{2.7a}$$

and

$$k_{rw} = S_e^{1/2} [1 - (1-S_e^{1/\gamma})^\gamma]^2 \tag{2.7b}$$

where n and γ are empirical parameters and S_e is the effective water saturation defined as $S_e = (S_w-S_{wr}) / (1-S_{wr})$ with S_{wr} being referred to as the residual water saturation.

The relationship of pressure head versus water saturation is described by the following function (van Genuchten, 1976; Mualem, 1976):

$$\frac{S_w - S_{wr}}{1 - S_{wr}} = \begin{cases} \dfrac{1}{[1+(\alpha|\psi-\psi_a|)^\beta]^\gamma} & \text{for } \psi < \psi_a \\ 1 & \text{for } \psi \geq \psi_a \end{cases} \tag{2.8}$$

where α and β are empirical parameters, and ψ_a is the air entry pressure head value. The parameters β and γ are normally related by $\gamma = 1\text{-}1/\beta$.

Equation (2.1) is solved using the Galerkin finite element subject to the initial and boundary conditions given in equations (2.5) and (2.6). After the distributions of ψ and S_w have been determined, the Darcy velocity is computed from

$$V_z = -Kk_{rw}\left(\frac{\partial \psi}{\partial z} - 1\right) \tag{2.9}$$

2.2.2 Solute Transport in Single-Phase Flow

The governing equation for one-dimensional transport of a nonconservative solute species in a variably saturated soil takes the form:

$$\frac{\partial}{\partial z}\left(D\,\frac{\partial c}{\partial z}\right) - V_z\,\frac{\partial c}{\partial z} = \theta R\left(\frac{\partial c}{\partial t} + \lambda c\right) \tag{2.10}$$

where D is the apparent hydrodynamic dispersion coefficient, c is the solute concentration, θ is the volumetric water content ($\theta = \phi S_w$), R is the retardation coefficient, and λ is the first-order decay constant.

The hydrodynamic dispersion D is computed using the following relationship:

$$D = \alpha_L V + D_w^* \tag{2.11}$$

where α_L is the longitudinal dispersivity, V is the absolute value of Darcy's velocity, V_z, and D_w^* is the apparent molecular diffusion in the water-phase.

$$D_w^* = (\tau\phi S_w^n) D_{mw} \tag{2.12}$$

in which τ is the tortuosity factor, D_{mw} is the free-water molecular diffusion coefficient, and n is an exponent parameter. Note that (2.12) corresponds to the Millington-Quirk equation if τ and n are set equal to $\phi^{1/3}$ and 10/3, respectively.

The initial and boundary conditions of the one-dimensional transport problem may be expressed as

$$c(z, 0) = c_i \tag{2.13}$$

and

$$c(z_B, t) = \tilde{c} \tag{2.14a}$$

or

$$-D\frac{\partial c}{\partial z}(z_B, t) = V_z(c_o - c) \tag{2.14b}$$

where c_i is the initial concentration, $\tilde{c}$ is the concentration at boundaries, and c_o is the leachate concentration at the source.

2.3 GOVERNING AND SUPPLEMENTARY EQUATIONS FOR MULTIPHASE MODELS

The multiphase components of SAMFT1D are formulated based upon immiscible flow equations (one equation for each active phase), and a single-species solute transport equation. These equations are described in this section together with initial and boundary conditions as well as other relevant supplementary constitutive relations.

2.3.1 Multiphase Flow

2.3.1.1 Flow Models

Consider a general situation involving flow of three active fluid phases, water, NAPL (NonAqueous Phase Liquid), and air or vapor. The governing equations of mass balance for the three phases may be expressed as follows:

water conservation:

$$\frac{\partial}{\partial z}\left[\frac{\rho_w k k_{rw}}{\mu_w}\frac{\partial \Phi_w}{\partial z}\right] + \rho_w q_w' = \frac{\partial}{\partial t}(\phi \rho_w S_w) \tag{2-15}$$

NAPL conservation:

$$\frac{\partial}{\partial z}\left[\frac{\rho_n k k_{rn}}{\mu_n}\frac{\partial \Phi_n}{\partial z}\right] + \rho_n q_n' = \frac{\partial}{\partial t}(\phi \rho_n S_n) \tag{2.16}$$

and air conservation:

$$\frac{\partial}{\partial z}\left[\frac{\rho_a k k_{ra}}{\mu_a}\frac{\partial \Phi_a}{\partial z}\right] + \rho_a q_a' = \frac{\partial}{\partial t}(\phi \rho_a S_a) \tag{2.17}$$

where:

ρ_ℓ = fluid density of phase ℓ (ℓ =w,n or a)

k = intrinsic permeability, function of the coordinate, z

$k_{r\ell}$ = relative permeability to phase ℓ

μ_ℓ = dynamic fluid viscosity of phase ℓ

q'_ℓ = volumetrical source/sink terms for phase ℓ

ϕ = porosity

S_ℓ = saturation of phase ℓ

and subscript ℓ=w=1, for water, ℓ=n=2, for NAPL, and ℓ=a=3, for air, and $\frac{\partial \Phi_\ell}{\partial z}$ is the component of potential gradient of phase ℓ in the z coordinate, defined as:

$$\frac{\partial \Phi_\ell}{\partial z} = \frac{\partial P_\ell}{\partial z} - \rho_\ell g \tag{2.18}$$

The constraint conditions are:

$$S_w + S_n + S_a = 1 \tag{2.19}$$

$$P_w = P_n - \bar{P}_{cnw}(S_w) \tag{2.20a}$$

and

$$P_a = P_n + \bar{P}_{can}(S_a) \tag{2.20b}$$

Typical relations for capillary pressure functions $\bar{P}_{cnw}$ and $\bar{P}_{can}$ are given by (Forsyth, 1990):

$$\bar{P}_{cnw} = \hat{\alpha} P_{cnw}(S_w) + (1 - \hat{\alpha}) P_{cnw}(S_w = 1) \tag{2.21a}$$

and

$$\bar{P}_{can} = \hat{\alpha} P_{can}(S_a) + (1 - \hat{\alpha}) [P_{caw}(S_a) - P_{cnw}(S_w = 1)] \tag{2.21b}$$

where $\hat{\alpha}$ = min (1, S_n/S_n^*), and S_n^* is critical NAPL saturation (Forsyth, 1990). Physically, S_n^* should be selected to be less than or equal to the minimum of the irreducible NAPL saturation for the water-NAPL and the NAPL-air fluid systems. $P_{cnw}(S_w)$ denotes capillary pressure between NAPL and water phases in the water-NAPL two-phase system as a function of water saturation, $P_{can}(S_a)$ denotes capillary pressure between air and NAPL phases in the NAPL-air two-phase system as a function of air saturation, and P_{caw} (S_a) denotes capillary pressure between air and water phases in the air and water two-phase system.

The six unknowns to be solved are: P_w, P_n, P_a, S_w, S_n and S_a. They can be determined using equations (2.15) - (2.17) and (2.19), (2.20a) and (2.20b). The primary dependent variables for the one-dimensional three-phase flow problem are chosen as P_n, S_w and S_n. In terms of the primary variables, the other three dependent variables may be expressed as:

$$S_a = 1 - S_w - S_n \tag{2.22}$$

$$P_w = P_n - \bar{P}_{cnw}(S_w) \tag{2.23}$$

and

$$P_a = P_w + \bar{P}_{cnw}(S_w) + \bar{P}_{can}(S_a) \tag{2.24}$$

2.3.1.2. Constitutive Relations

(a) Capillary Pressure

The capillary pressure functions are needed in multiphase flow simulations to relate the pressures between all the phases. The capillary pressure curves are normally experimentally determined as functions of water or air saturations,

$$P_{cnw} = P_{cnw}(S_w) \tag{2.25}$$

and

$$P_{can} = P_{can}(S_a) \tag{2.26}$$

for NAPL-water and air-NAPL two phase systems, respectively. However, when dealing with multiphase contamination problems in soil and groundwater systems, the NAPL phase may not exist in the entire or certain parts of the flow domain initially or during the time period of simulation. We also need the capillary pressure curve between air and water phases:

$$P_{caw} = P_{caw}(S_a) \tag{2.27}$$

The phase pressure relations including smooth transition of two phases (water-air) to three phases (water-NAPL-air) during simulations are described (Forsyth, 1990) as

$$\bar{P}_{cnw} = P_n - P_w = \hat{\alpha} P_{cnw}(S_w) + (1 - \hat{\alpha}) P_{cnw}(S_w = 1) \tag{2.28}$$

$$\bar{P}_{can} = P_a - P_n = \hat{\alpha} P_{can}(S_a) + (1 - \hat{\alpha}) \left[P_{caw}(S_a) - P_{cnw}(S_w = 1) \right] \tag{2.29}$$

and

$$\begin{aligned} P_a - P_w &= \bar{P}_{can} + \bar{P}_{cnw} \\ &= \hat{\alpha} \left[P_{cnw}(S_w) + P_{can}(S_a) \right] + (1 - \hat{\alpha}) P_{caw}(S_a) \end{aligned} \tag{2.30}$$

(b) Relative Permeability

The three-phase relative permeability functions used are:

Relative permeability to water phase,

$$k_{rw} = k_{rw}^{wn}(S_w) \tag{2.31}$$

relative permeability to air phase,

$$k_{ra} = k_{ra}^{na}(S_a) \tag{2.32}$$

and relative permeability to NAPL phase,

$$k_{rn} = k_{rn}(S_w, S_n) \tag{2.33}$$

which are also computed from two sets of experimentally determined functions: k_{rw}^{wn}, water relative permeability, from an oil-water system, and air relative permeability k_{ra}^{na} from an oil-air system. k_{rn} is calculated by the Stone model 2, (Aziz and Settari, 1979),

$$k_{rn}(S_w, S_a) = k_{rn}^{*wn}\left[(k_{rn}^{wn}/k_{rn}^{*wn} + k_{rw})\,(k_{rn}^{na}/k_{rn}^{*wn} + k_{ra}) - (k_{rw} + k_{ra})\right] \tag{2.34}$$

with the constraint

$$k_{rn} \geq 0 \tag{2.35}$$

where k_{rn}^{*wn} is the relative permeability to NAPL phase at irreducible water saturation in a water-NAPL two-phase system.

(c) Functional Relations of Capillary Pressure and Relative Permeability

The SAMFT1D code has provided the user with an additional option of using functional forms of constitutive relations, when no tabulated experimental data are available. For capillary pressures, these relations may be obtained using the equation scaling procedure described by Lenhard and Parker (1987). The scaled van Genuchten constitutive relation applicable to a given pair of wetting and non-wetting fluids is first expressed as

$$\tilde{S} = \left[1 + (\alpha\tilde{h})^{\beta}\right]^{-\gamma} \tag{2.36}$$

where $\tilde{S}$ is the effective wetting phase saturation corresponding to a scaled value of capillary pressure head $\tilde{h}$, and $\gamma = 1 - 1/\beta$.

Equation (2.36) may be rearranged to give

$$\tilde{h} = \frac{1}{\alpha}\left[(1/\tilde{S})^{1/\gamma} - 1\right]^{1/\beta} \tag{2.37}$$

For the three-phase (w-n-a) system, equation (2.37) is applied to the three fluid pairs, w-n, a-n and a-w. This leads to the following set of constitutive relations in terms of pressures and saturations:

$$P_{cnw} = \frac{\sigma_{nw}\rho_{fw}g}{\alpha\,\sigma_{aw}}\left[\left(\bar{S}_w\right)^{-1/\gamma} - 1\right]^{1/\beta} \tag{2.38}$$

$$P_{can} = \frac{\sigma_{an}\rho_{fw}g}{\alpha\,\sigma_{aw}}\left[\left(1 - \bar{S}_a\right)^{-1/\gamma} - 1\right]^{1/\beta} \tag{2.39}$$

and

$$P_{caw} = \frac{\rho_{fw}g}{\alpha}\left[\left(1 - \bar{S}_a\right)^{-1/\gamma} - 1\right]^{1/\beta} \tag{2.40}$$

where

$$\bar{S}_w = \frac{S_w - S_{wr}}{1 - S_{wr}}$$

and

$$\bar{S}_a = \frac{S_a}{1 - S_{wr}}$$

In Eqs. (2.38) - (2.40) σ_{nw}, σ_{an}, and σ_{aw} are interfacial tensions between NAPL, water, and air phases, respectively, and ρ_{fw} is the density of fresh-water. Equations (2.38) - (2.40) need to be used in conjunction with the pressure relations given in equations (2.28) - (2.30) to ensure continuity when the NAPL phase first appears or disappears.

For relative permeability, two forms of functions are used in the code, as follows:

(i) van Genuchten's Relative Permeability Functions

The following functions given by Parker (1989) may be used for three-phase relative permeabilities:

$$k_{rw} = (\bar{S}_w)^{1/2} \left\{1 - \left[1 - (\bar{S}_w)^{1/\gamma}\right]^{\gamma}\right\}^2 \tag{2.41}$$

$$k_{rn} = (\bar{S}_n - \bar{S}_{nr})^{1/2} \left\{\left[1 - (\bar{S}_w)^{1/\gamma}\right]^{\gamma} - \left[1 - (\bar{S}_L)^{1/\gamma}\right]^{\gamma}\right\}^2 \tag{2.42}$$

and

$$k_{ra} = (\bar{S}_a)^{1/2} \left[1 - (\bar{S}_L)^{1/\gamma}\right]^{2\gamma} \tag{2.43}$$

where

$$\bar{S}_n = \frac{S_n}{1 - S_{wr}}$$

$$\bar{S}_L = \bar{S}_n + \bar{S}_w$$

and

$$\bar{S}_{nr} = \frac{S_{nr}}{1 - S_{wr}}$$

and S_{nr} is the residual NAPL saturation.

(ii) Brooks-Corey Relative Permeability Functions

Alternatively, the Brooks-Corey Functions (Honapour, et. al, 1986) may be used in conjunction with Stone's procedure to evaluate relative permeabilities for three-phase system:

$$k_{rw} = k_{rw}^{wn}(\bar{S}_w) = (\bar{S}_w)^{N+2} \tag{2.44}$$

$$k_{rn} = (\bar{S}_n - \bar{S}_{nr})^2 \left[(\bar{S}_L)^N - (\bar{S}_w)^N\right] \tag{2.45}$$

and

$$k_{ra} = k_{ra}^{na}(\bar{S}_a) = (\bar{S}_a)^2 \left[1 - (\bar{S}_L)^N\right] \tag{2.46}$$

where N = 1+2/n with n being referred to as the Brooks-Corey pore size distribution parameter.

(d) Two-Phase Constitutive Relations

For a special case of a given pair of two-phase fluids, the two-phase capillary pressure and relative permeability can be obtained from the above three-phase correlations depending on the fluid pair specification. The capillary pressure curves are elected from equations (2.28), (2.29) and (2.30). The relative permeability functions are from equations (2.31) and (2.32) for

tabulated data and from equations (2.41) and (2.43), or (2.44) and (2.46) for functional forms, respectively, with the air phase replaced by the non-wetting phase.

(e) Equations of State

The densities of the three fluid phases are prescribed as functions of the pressure of each phase as:

$$\rho_w = \rho_w^o \, e^{C_w (P_w - P_o)} \approx \rho_w^o \left[1 + C_w \, (P_w - P_o)\right] \tag{2.47}$$

$$\rho_n = \rho_n^o \, e^{C_n (P_n - P_o)} \approx \rho_n^o \left[1 + C_n \, (P_n - P_o)\right] \tag{2.48}$$

$$\rho_a = \frac{P_a M}{RT} = C_a \, P_a \tag{2.49}$$

and porosity is described by,

$$\phi = \phi(P_w) \approx \phi_o \left[1 + C_r \, (P_w - P_o)\right] \tag{2.50}$$

where

P_o = reference pressure

ρ_w° = water density at $P_w = P_o$

ρ_n° = NAPL density at $P_n = P_o$

$C_w = \left. \frac{1}{\rho_w} \frac{\partial \rho_w}{\partial P_w} \right|_T$, water compressibility

$C_n = \left. \frac{1}{\rho_n} \frac{\partial \rho_n}{\partial P_n} \right|_T$, NAPL compressibility

C_a = $\frac{M}{RT}$, air compressibility factor

M = Molecular weight of the gas phase

R = Universal gas constant

T = Constant (absolute) temperature

C_r = $\frac{1}{\phi}\left.\frac{\partial \phi}{\partial P_w}\right|_T$, rock or soil volume compressibility

ϕ_o = Porosity at $P_w = P_o$, function of the coordinate z.

2.3.1.3 Initial and Boundary Conditions

The initial conditions needed for solving the multiphase flow equations (2.15) - (2.17) are:

$$p_w(z, 0) = P_i(z) \tag{2.51}$$

$$S_w(z, 0) = S_{wi}(z) \tag{2.52}$$

and

$$S_n(z, 0) = S_{ni}(z) \tag{2.53}$$

where $P_i(z)$, $S_{wi}(z)$ and $S_{ni}(z)$ are the initial water phase pressure and saturation, and NAPL saturation, respectively, as functions of the coordinate z.

The boundary conditions to be specified are either prescribed phase pressure or phase flux conditions at the top or bottom boundaries. The top boundary conditions are treated as injection or source terms,

$$P_\ell(0,\ t) = P_\ell^o(t) \qquad (\ell = w,\ n\ or\ a) \tag{2.54}$$

or

$$q_\ell = q_\ell^o(t) \qquad (\ell = w,\ n\ or\ a) \tag{2.55}$$

where $P_\ell^o(t)$ and $q_\ell^o(t)$ are prescribed injection pressure and flux of phase ℓ, respectively, as functions of time. If only one phase injection pressure is specified on the top boundary, the code will set the pressures of all the other phases equal to the specified one. The bottom boundary is regarded as a production (sink) boundary with pressure or flux specified, for pressure conditions:

$$P_\ell(H,\ t) = P^B(t) \qquad (\ell = w,\ n,\ a) \tag{2.56}$$

or for sink terms:

$$q_T = q_T^B(t) \tag{2.57}$$

where H is the coordinate of the bottom boundary, $P^B(t)$ is bottom boundary pressure, and $q_T^B(t)$ is total liquid mass production rate, respectively, as functions of time.

2.3.2 Solute Transport in Multiphase Flow

2.3.2.1 Transport Model

The equation describing transport of a non-conservative solute component in a fluid phase ℓ (ℓ = w,n,a) may be written in the form:

$$\frac{\partial}{\partial z}\left[D_\ell \frac{\partial}{\partial z}(\rho_\ell c_\ell)\right] - \frac{\partial}{\partial z}(V_\ell \rho_\ell c_\ell) = \frac{\partial}{\partial t}(\phi S_\ell \rho_\ell c_\ell) + \lambda_\ell \phi S_\ell \rho_\ell c_\ell + Q_\ell \rho_\ell (c_\ell - c_\ell^*) - \Gamma_\ell \tag{2.58}$$

where c_ℓ is mass fraction concentration of the component concerned in fluid phase ℓ (defined as mass of the solute per unit mass of fluid phase ℓ), ρ_ℓ is the fluid density, D_ℓ is the apparent hydrodynamic dispersion coefficient with respect to fluid phase ℓ, V_ℓ is the Darcy velocity of fluid phase ℓ, λ_ℓ is the decay coefficient in fluid phase ℓ, Q_ℓ is the volumetric rate of fluid injection per unit bulk volume of the porous medium, and c_ℓ^* is the injected solute concentration in phase ℓ and Γ_ℓ is the net rate of solute mass transfer into or out of phase ℓ per unit volume of the porous medium.

The net mass transfer rate, Γ_ℓ, accounts for the component mass transfer between phase ℓ and each of the remaining fluid phases as well as the component mass transfer between phase ℓ and a "precipitated phase" of the solute component. This "precipitated phase" is an immobile phase allowed to occur in our conceptual model when the dissolved concentration exceeds the solubility limit. In treating the multiphase flow equations, we have assumed that the net effect of contaminant mass transfer between various fluid phases is negligible. This assumption is valid if the component concerned is slightly soluble.

By expanding the advection and mass accumulation terms and enforcing the continuity requirement for fluid flow, equation (2.58) may be expressed in the form:

$$\frac{\partial}{\partial z}\left[D_\ell \rho_\ell \frac{\partial c_\ell}{\partial z}\right] - V_\ell \rho_\ell \frac{\partial c_\ell}{\partial z} = \phi S_\ell \rho_\ell \frac{\partial c_\ell}{\partial t} + \lambda_\ell \phi S_\ell \rho_\ell c_\ell + Q_\ell \rho_\ell (c_\ell - c_\ell^*) - \Gamma_\ell \tag{2.59}$$

where the term $\frac{\partial}{\partial z}\left[D_\ell c_\ell \frac{\partial \rho_\ell}{\partial z}\right]$ has been neglected, and the following fluid continuity equation has been used:

$$-\frac{\partial}{\partial t}(V_\ell \rho_\ell) = \frac{\partial}{\partial t}(\phi S_\ell \rho_\ell) \tag{2.60}$$

The mass balance equation for the precipitated phase (assumed to be immobile) is given by

$$\frac{\partial}{\partial t}(\rho_p S_p \phi) + \lambda_p \phi \rho_p S_p = \Gamma_p \tag{2.61}$$

where ρ_p, S_p and λ_p are density, saturation, and decay coefficient of the precipitated contaminant phase, and Γ_p is the net rate of mass transfer between the precipitated phase and all other remaining fluid and solid phases.

The equation describing solute mass distribution in the porous matrix is given by

$$\frac{\partial}{\partial t}[(1-\phi)\rho_s c_s] + (1-\phi)\rho_s \lambda_s c_s = \Gamma_s \tag{2.62}$$

where c_s and λ_s are the solute concentration and the coefficient of decay in the solid phase, respectively, ρ_s is the density of the solid porous material, and Γ_s is the rate of solute mass

transfer between the soil matrix and all other phases. Equation (2.59) may be summed with respect to all fluid phases (w,n,a) and combined with (2.60), (2.61) and (2.62) to give

$$\sum_{\ell} \left[\frac{\partial}{\partial z} \left[D_\ell \rho_\ell \frac{\partial c_\ell}{\partial z} \right] - V_\ell \rho_\ell \frac{\partial c_\ell}{\partial z} \right] = \sum_{\ell} \left(\phi S_\ell \rho_\ell \frac{\partial c_\ell}{\partial t} \right.$$

$$\left. + \lambda_\ell \phi S_\ell \rho_\ell c_\ell \right) + (1 - \phi) \rho_s \left[\frac{\partial c_s}{\partial t} + \lambda_s c_s \right] + \sum_{\ell} \rho_\ell Q_\ell (c_\ell - c_\ell^*) \qquad (2.63)$$

$$+ \frac{\partial}{\partial t} \left[\rho_p S_p \phi \right] + \lambda_p \phi \rho_p S_p$$

where the following mass-conservation constraint has been applied:

$$\Gamma_w + \Gamma_n + \Gamma_a + \Gamma_s + \Gamma_p = 0 \qquad (2.64)$$

and the component concentration in the precipitated phase is considered to be unity.

The partitioning of solute mass between different phases is described by means of linear equilibrium isotherms. Since these isotherms are linear, the partitioning relations required for transport in three-phase flow may be expressed using water as the reference phase as follows:

$$c_n = \kappa_n c_w \, H(S_n) \qquad (2.65a)$$

$$c_a = \kappa_a c_w \, H(S_a) \qquad (2.65b)$$

$$c_s = k_d \rho_w c_w \qquad (2.65c)$$

where κ_n, κ_a and k_d are partitioning coefficients relating concentration in the water phase to concentrations in the nonaqueous phase, the air phase and the solid phase, respectively, and $H(\xi)$ is the Heaviside step function where $H(\xi) = 0$ for $\xi \leq 0$ and $= 1$ for $\xi > 0$. The Heaviside function is used to designate the fact that c_n and c_a are zero when NAPL and air saturations are

zero. Note that κ_n and κ_a are dimensionless and k_d is a distribution coefficient having a dimension of volume per unit mass.

The air-water partitioning coefficient, κ_a, is generally known as Henry's constant. The NAPL-water partitioning coefficient, κ_n, may be expressed as

$$\kappa_n = \kappa_a / \kappa_a^* \tag{2.66}$$

where κ_a^* is the air-NAPL partitioning coefficient known as Raoult's constant.

Equation (2.63) can be combined with (2.65a)-(2.65c) to give the following equation:

$$\begin{aligned} \frac{\partial}{\partial z}\left[(D_w\rho_w + \kappa_n\rho_n D_n + \kappa_a\rho_a D_a)\frac{\partial c_w}{\partial z}\right] \\ - (V_w\rho_w + \kappa_n\rho_n V_n + \kappa_a\rho_a V_a)\frac{\partial c_w}{\partial z} = \phi(RS_w\rho_w + \kappa_n S_n\rho_n + \kappa_a S_a\rho_a)\frac{\partial c_w}{\partial t} \\ + \phi\lambda(RS_w\rho_w + \kappa_n S_n\rho_n + \kappa_a S_a\rho_a)c_w \\ + \sum_\ell \rho_\ell Q_\ell (c_\ell - c_\ell^*) + \frac{\partial}{\partial t}[\rho_p \phi S_p] \\ + \lambda_p \phi \rho_p S_p \end{aligned} \tag{2.67}$$

where R is given by

$$R = 1 + \frac{(1-\phi)\rho_s k_d}{\phi S_w} \tag{2.68}$$

and it has been assumed that $\lambda_\ell = \lambda_s = \lambda$.

We now introduce the following definitions:

$$D_T = \rho_w D_w + \rho_n \kappa_n D_n + \rho_a \kappa_a D_a \tag{2.69}$$

$$V_T = \rho_w V_w + \rho_n \kappa_n V_n + \rho_a \kappa_a V_a \tag{2.70}$$

$$R_T = R\rho_w S_w + \kappa_n \rho_n S_n + \kappa_a \rho_a S_a \tag{2.71}$$

$$Q_T = \rho_w Q_w + \rho_n Q_n \kappa_n + \rho_a Q_a \kappa_a \tag{2.72}$$

$$(Qc)_T^* = \rho_w Q_w C_w^* + \rho_n Q_n C_n^* + \rho_a Q_a C_a^* \tag{2.73}$$

Equation (2.67) may be combined with (2.69) - (2.73) to give the following governing equation:

$$\frac{\partial}{\partial z}\left[D_T \frac{\partial c_w}{\partial z}\right] - V_T \frac{\partial c_w}{\partial z} = \phi R_T \left(\frac{\partial c_w}{\partial t} + \lambda c_w\right) + \frac{\partial}{\partial t}[m_p] + \lambda_p m_p + Q_T c_w - (Qc)_T^* \tag{2.74}$$

where $m_p = \phi \rho_p S_p$.

Equation (2.74) needs to be solved numerically subject to the following constraints:

$$c_w \leq c_{ws} \tag{2.75}$$

and

$$m_p \geq 0 \tag{2.76}$$

where c_{ws} is the water-solubility limit (maximum dissolved concentration) of the component concerned.

2.3.2.2. Supplementary Equations

Note that the Darcy velocity and hydrodynamic dispersion for each fluid phase are computed using the following relations:

$$V_\ell = - \frac{k k_{r\ell}}{\mu_\ell} \frac{\partial \Phi_\ell}{\partial z} \tag{2.77}$$

$$D_\ell = \alpha_L |V_\ell| + (\phi \tau^* S_\ell^n) D_{m\ell} \tag{2.78}$$

where α_L is the longitudinal dispersivity, $D_{m\ell}$ is free-fluid molecular diffusion coefficient for fluid phase ℓ, τ^* is tortuosity factor, and n is an exponent. If the Millington-Quirk expression is to be used, then N and τ^* are set equal to 10/3 and $\phi^{1/3}$, respectively.

For a passive fluid phase, it is assumed that $V_\ell = 0$.

2.3.2.3 Initial and Boundary Conditions

The initial and boundary conditions associated with the multiphase solute transport equation may be expressed as

$$c_w(x_i, 0) = c_w(x_i) \tag{2.79}$$

and

$$c_w(x_i, t) = \bar{c}_w \text{ on } B_1' \tag{2.80a}$$

or

$$D_T \frac{\partial c_w}{\partial z} = \dot{m}_D \text{ on } B_2' \tag{2.80b}$$

or

$$D_T \frac{\partial c_w}{\partial z} - V_T c_w = \dot{m}_T \text{ on } B_3' \qquad (2.80c)$$

where B_1' is the boundary portion where the solute concentration in the water phase is prescribed c_w, B_2' is the boundary portion where dispersive mass flux of solute is prescribed as $\dot{m}_D$, and B_3' is the boundary portion where the total solute mass flux is prescribed as $\dot{m}_T$. Note that the sign conventions for $\dot{m}_D$ and $\dot{m}_T$ are positive for influx and negative for efflux.

2.4 ASSUMPTIONS

In this section, major assumptions incorporated into the single-phase and multiphase mathematical models are provided.

2.4.1 Single-Phase Models

Major assumptions of the single-phase flow model of SAMFT1D are as follows:

- Water is the only active phase (i.e., other fluid phases assumed to be passive)
- Flow of the water-phase is considered isothermal and governed by Darcy's law
- The active fluid phase is slightly compressible and homogeneous
- The soil or rock medium may be represented by a single-continuum porous medium.

Major assumptions of the single-phase solute transport model are as follows:

- Transport in the porous medium system is governed by Fick's law. The hydrodynamic dispersion coefficient is defined as the sum of the coefficients of mechanical dispersion and molecular diffusion

- Adsorption and decay of the solute may be described by a linear equilibrium isotherm and a first order decay constant.

2.4.2 Multiphase Models

Major assumptions of the multiphase flow model are as follows:

- Flow of each phase may be treated as isothermal and governed by Darcy's law
- Both liquid phases (water and NAPL) are slightly compressible and homogeneous
- The compressible air phase may be treated as an ideal gas
- The soil or rock medium may be represented by a single-continuum porous medium.

Major assumptions of the multiphase solute transport model are as follows:

- Transport in the porous medium system is governed by Fick's law. The hydrodynamic dispersion coefficient is defined as the sum of the coefficients of mechanical dispersion and molecular diffusion
- Adsorption and decay of the solute may be described by a linear equilibrium isotherm and a first order decay constant
- Partitioning of solute mass between different phases is described by means of linear equilibrium isotherms, and solute concentration is subject to the water-solubility limit.

2.5 LIMITATIONS

The SAMFT1D code has the following limitations:

- In performing single-phase or multiphase flow analysis, the code neglects effects of temperature variation and non-Darcian or non-Newtonian behavior of the fluids

- The code considers only single-porosity soil or aquifer media. It cannot handle fractured media or structured soils

- In performing solute transport analysis, the code does not take into account sorption nonlinearity or kinetic effects which, in some instances, can be important. Furthermore, effects of changes in fluid properties due to variations in solute concentrations are neglected. Solute mass transfer between fluid phases (other than the partitioning between phases by Henry's law) is also neglected.

2.6 INPUT DATA

Input data and parameters required by the single-phase and multiphase models of SAMFT1D are summarized below. A full description of data requirements is provided in Chapter 8.

2.6.1 Single-Phase Models

Input data and parameters for variably saturated flow simulations include the following:

(1) System Geometry

- Horizontal and vertical dimensions including layering and other heterogeneities (L)

(2) Porous Medium Properties

- Intrinsic permeability, k (L^2)
- Volume compressibility, C_r (LT^2/M)
- Effective porosity, ϕ

(3) Fluid Properties

- Density of water, ρ_w (ML^{-3})
- Dynamic viscosity of water, μ_w ($ML^{-1}\ T^{-1}$)

- Volume compressibility of water, C_w (LT^2/M)

(4) Capillary Pressure and Relative Permeability

- Coefficient of van Genuchten function, α (L^{-1})
- Power index of van Genuchten function, β, γ
- Exponent of Brooks-Corey function, N

(5) Initial and Boundary Conditions

- Initial distribution of water-phase pressure, P_w, potential, Φ_w, or saturation, S_w ($ML^{-1}\ T^{-2}$)
- Prescribed values of P_w at specified Dirichlet boundary nodes ($ML^{-1}\ T^{-2}$)
- Prescribed values of water fluxes at specified flux nodes ($ML^{-1}\ T^{-1}$)

Input data and parameters for the transport model include the following:

(1) System Geometry

- Horizontal and vertical dimensions including layering and other heterogeneities (L)

(2) Porous Medium Properties

- Longitudinal dispersivity, α_L (L)
- Apparent molecular diffusion coefficient, D^* ($L^2\ T^{-1}$)
- Effective porosity, ϕ
- Bulk density, ρ_B (ML^{-3})

(3) Properties of Solute Species

- Decay coefficient, λ (T^{-1})
- Distribution coefficient, k_d ($L^3 M^{-1}$)

(4) Darcy velocity of water phase (LT^{-1})

(5) Saturation of the fluid phase considered, S_w

(6) Initial and boundary conditions

- Initial distribution of concentration, c_o (ML^{-3})
- Prescribed values of concentration, $\tilde{c}$ (ML^{-3})
- Prescribed values of solute flux, $\dot{m}$ (MT^{-1})

(7) Fluid flux data at the boundary nodes (LT^{-1})

2.6.2 Multiphase Models

Input data and parameters for multiphase flow and transport simulations are similar to those for single-phase flow and transport except that reference is now made to each active fluid phase. Tabulated or functional relationships are used to describe the relative permeabilities of various fluid phases and capillary behavior. A full description of data requirements is provided in Chapter 8.

Input data and parameters for multiphase flow simulations include the following:

(1) System Geometry

- Horizontal and vertical dimensions including layering and other heterogeneities (L)

(2) Porous Medium Properties

- Intrinsic permeability, k (L^2)
- Volume Compressibility, C_r (LT^2/M)

- Effective porosity at atmospheric pressure, ϕ_o.

(3) Fluid Properties

- Fluid densities of all the phases at atmospheric pressure, ρ_ℓ^o (ℓ = w, n, and a) (ML^{-3})
- Dynamic viscosity of all the phases, μ_ℓ (ℓ = w, n and a) ($ML^{-1}\ T^{-1}$)
- Liquid compressibility, C_ℓ (ℓ = w and n) (LT^2/M)
- Air compressibility, C_a (T^2/L^2)

(4) Capillary pressure and relative permeability

Tabulated Data:

- Phase saturation and capillary pressure data
- Phase saturation and relative permeability data

Functional relations:

- Coefficient of van Genuchten function, α (L^{-1})
- Power index of van Genuchten function, β, γ
- Exponent of Brooks-Corey function, N
- Interfacial surface tensions between distinct phases, σ_{aw}, σ_{nw}, and σ_{an} ($M\ T^{-2}$)

(5) Initial and Boundary Conditions

- Initial distribution of water-phase pressure, P_w, potential, Φ_w, or saturation S_w ($ML^{-1}\ T^{-2}$)
- Prescribed values of phase pressure P_ℓ (ℓ = w, n, or a) at specified Dirichlet boundary nodes ($ML^{-1}\ T^{-2}$)

- Prescribed values of fluid fluxes at specified flux nodes ($ML^{-2}\ T^{-1}$)

Input data and parameters for the multiphase transport model include the following:

(1) System Geometry

- Horizontal and vertical dimensions including layering and other heterogeneities (L)

(2) Porous Medium Properties

- Longitudinal dispersivity, α_L (L)
- Apparent molecular diffusion coefficient in all the fluid phases, D_ℓ^* ($L^2\ T^{-1}$)
- Effective porosity, ϕ
- Bulk density, ρ_B (ML^{-3})

(3) Properties of Solute Species

- Decay coefficient, λ (T^{-1})
- Distribution coefficient, k_d ($L^3\ M^{-1}$)
- Solubility limit in water phase, c_{ws}
- Partitioning coefficient between water and NAPL phases, κ_n
- Partitioning coefficient between NAPL and air phases, κ_a

(4) Darcy velocity of each fluid phase (LT^{-1})

(5) Saturation of each fluid phase considered, S_ℓ (ℓ = w, n, or a)

(6) Initial and boundary conditions

- Initial distribution of concentration, c_o (M/M)

- Initial distribution of precipitated mass (ML^{-3})
- Prescribed values of concentration on boundaries, $\tilde{c}$ (M/M)
- Prescribed values of solute flux on boundaries, $\dot{m}$ (MT^{-1})

(7) Fluid flux data at the boundary nodes ($ML^{-2}T^{-1}$)

2.7 OUTPUT FROM MODELS

2.7.1 Single-Phase Models

For a single-phase flow simulation, the primary line printer output includes nodal values of pressure or pressure head, Darcy velocity and water-phase saturation at specified time levels. The code allows the user to select its fluid volumetric balance calculation option. If this option is selected, a fluid volumetric balance budget will also be printed out at the end of each time step. This budget contains information about the net flow rate of fluid due to boundary fluxes, sources and sinks, the rate of fluid accumulation in the entire flow domain, the flow balance error, and the cumulative volumetric fluid storage up to the current time.

To enable the user to use results from the flow model to run the transport model, SAMFT1D also provides the main link of the two models by writing the linking information on FORTRAN Unit 9. This information includes computed element centroidal values of Darcy velocities and fluid saturation, nodal fluid storage terms, and boundary nodal flux values.

A restart option for the flow model is provided in the code. This is facilitated by writing the nodal values of pressure head computed at the final time step of the current run on FORTRAN Unit 8.

The primary line printer output of the transport model SAMFT1D includes nodal values (at user-selected time levels) of solute concentration. SAMFT1D also allows the user to select its solute mass balance calculation option. If this option is selected, a solute component mass balance budget will be printed at the end of each time step. This budget contains information about the total dispersive and advective fluxes, the net rate of material accumulation taking into account storage, adsorption and decay, the mass balance error, the cumulative mass of solute still remaining in the porous medium at the current time, and the cumulative mass decay up to the current time value.

A restart option for the transport model is also provided in the code. This is facilitated by writing the nodal values of concentration computed at the final time step of the current run on FORTRAN Unit 8.

The SAMFT1D code is also capable of performing combined flow/transport simulation or sequential simulations of flow and transport. In the concurrent simulation approach, the flow and transport equations are solved together in each time step. Thus there is no need to be concerned about creating velocity backup files for transport simulations. In the sequential simulation approach, the flow problem is solved for the entire time period of simulation. In order to solve the associated transport problem after running the flow problem, the user should select an option that directs the code to write values of element velocities and water saturation obtained by solving the flow problem onto FORTRAN Unit 9. The information written on Unit 9 should then be supplied to the code as supplementary input data for the transport calculation.

2.7.2 Multiphase Models

For a multiphase flow simulation, the primary line printer output includes nodal values of pressure and saturation of each fluid phase at specified time levels. The code allows the user to select its fluid mass balance calculation option. If this option is selected, a fluid mass balance budget will also be printed out at the end of each time step or required time steps. This budget contains information about the net flow rate of fluid due to boundary fluxes, sources and sinks, the rate of fluid accumulation in the entire flow domain, and the cumulative fluid mass balance errors up to the current time.

For transport modeling, the primary line printer output includes nodal values of solute concentrations in all the phases and precipitated solute mass. Similarly, to enable the user to use results from the multiphase flow model to run the multiphase transport model, SAMFT1D also provides the main link of the two models by writing the linking information on FORTRAN Unit 9. This information includes computed element centroidal values of Darcy velocities and fluid saturations of each fluid phase. The output organization and options for multiphase transport models are similar to those for single-phase models. Also for both flow and transport simulations of multiphase models restart options are provided in the code, and using procedures are the same as discussed in the previous section for single-phase models.

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3 NUMERICAL SOLUTION TECHNIQUES

3.1 GENERAL

In this chapter, numerical techniques for approximating the fluid flow and solute transport equations under single-phase and multiphase conditions are described. In the single-phase computational modules, the variably saturated water flow equation is treated using the Galerkin finite element method in conjunction with either the Picard or Newton-Raphson iterative scheme. In the multiphase computational modules, the governing equations for flow simulation are treated using block-centered finite difference approximation techniques with upstream weighting of phase mobilities. The transport equations for both single- and multi-phase conditions are treated using the upstream-weighted finite element method.

3.2 NUMERICAL TREATMENT OF SINGLE-PHASE FLOW AND TRANSPORT PROBLEMS

3.2.1 Variably Saturated Flow

A numerical approximation of the one-dimensional flow equation is obtained using a Galerkin finite element formulation (see Huyakorn and Pinder, 1983) with spatial discretization performed using linear elements. Time integration is performed using a backward finite difference approximation. This leads to a system of nonlinear algebraic equations. For a typical node i in the finite element grid (see Figure 3.1), the equation may be expressed as

$$\alpha_i \psi_{i-1}^{k+1} + \beta_i \psi_i^{k+1} + \gamma_i \psi_{i+1}^{k+1} = d_i \qquad (3.1)$$

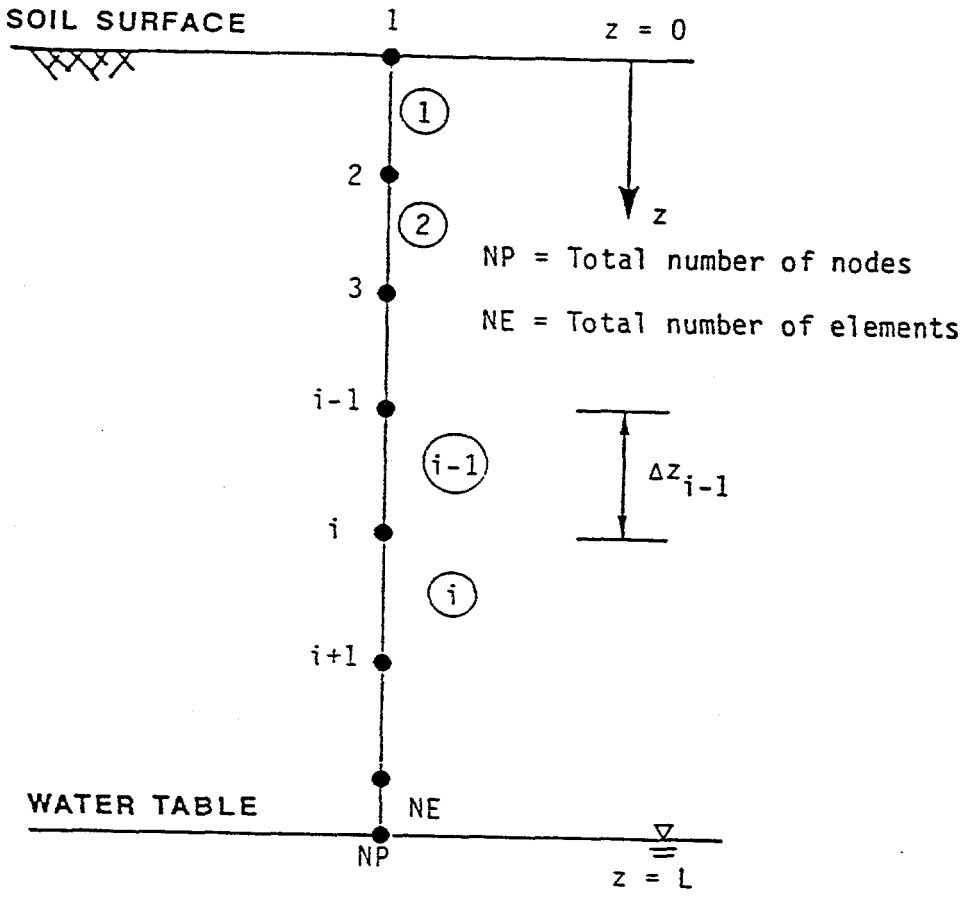

Figure 3.1. Finite element discretization of soil column showing node and element numbers.

where k+1 is the current time level, and α_i, β_i, γ_i, and d_i are given by

$$\alpha_i = \frac{-<Kk_{rw}>_{i-1}}{\Delta z_{i-1}} \tag{3.2a}$$

$$\beta_i = \frac{<Kk_{rw}>_{i-1}}{\Delta z_{i-1}} + \frac{<Kk_{rw}>_i}{\Delta z_i} + \frac{\eta_i}{\Delta t_k} \tag{3.2b}$$

$$\gamma_i = \frac{-<Kk_{rw}>_i}{\Delta z_i} \tag{3.2c}$$

$$d_i = \left[\frac{\eta_i}{\Delta t_k}\right] \psi_i^k + <Kk_{rw}>_{i-1} - <Kk_{rw}>_i \tag{3.2d}$$

where Δz_i and Δt_k are the spatial and time increments, respectively. Note that angular brackets are used to denote the value of the enclosed quantity at the element centroid. The nonlinear system of equations is solved for each time step. Two nonlinear schemes are provided in the code. The first scheme is a Picard type iteration scheme and the second is a Newton-Raphson scheme.

In the Picard scheme, the matrix coefficients, α_i, β_i, γ_i, and d_i, are first evaluated using an initial estimate of pressure head values, ψ_i^k. The resulting system of linearized equations is then solved for ψ_i^{k+1} using the Thomas algorithm. Updating of the matrix coefficient is performed by recomputing values of nonlinear soil parameters. Iterations are performed until the successive change in pressure head values is within a prescribed tolerance.

In the Newton-Raphson scheme, the nonlinear system of equations is treated by applying the Newton-Raphson technique (see Huyakorn and Pinder, 1983, pp. 159-162) to equation (3.1). This leads to the following system of linearized algebraic equations:

$$(\alpha_i + \alpha_i^*)^r \psi_{i-1}^{k+1} + (\beta_i + \beta_i^*)^r \psi_i^{k+1} + (\gamma_i + \gamma_i^*)^r \psi_{i+1}^{k+1} = (d_i + d_i^*)^r \tag{3.3}$$

where superscript r is used to denote the r-th iterate, α_i, β_i, γ_i, and d_i are as defined previously, and α_i^*, β_i^*, γ_i^*, and d_i^* are given by

$$\alpha_i^* = 1/2 \left[-1 + \frac{(\psi_i - \psi_{i-1})^r}{\Delta z_{i-1}} \right] < K \frac{dk_{rw}}{dS_w} \frac{dS_w}{d\psi} >_{i-1}^r \tag{3.4a}$$

$$\beta_i^* = \alpha_i^* + \gamma_i^* + \frac{\eta_i}{\Delta t_k} \left[\frac{\partial \eta_i}{\partial \psi_i} \right]^r \tag{3.4b}$$

$$\gamma_i^* = 1/2 \left[1 + \frac{(\psi_i - \psi_{i+1})^r}{\Delta z_i} \right] < K \frac{dk_{rw}}{dS_w} \frac{dS_w}{d\psi} >_i \tag{3.4c}$$

$$d_i^* = \alpha_i^* \psi_{i-1}^r + \beta_i^* \psi_i^r + \gamma_i^* \psi_{i+1}^r \tag{3.4d}$$

The initial solution and subsequent iterations of the Newton-Raphson scheme are performed in the same manner as that described for the Picard scheme.

In designing a finite element grid for variably saturated flow simulations, one should select nodal spacings that will yield reasonable approximations to the expected moisture profiles. In the analysis of the given variably saturated flow problem, small nodal spacings should be used in the zones where head gradients or moisture fronts are steep. The nodal spacings may be gradually increased in the zone where no abrupt changes in hydraulic conductivities occur and the head gradients are gradually sloping. The variably saturated flow simulation can be performed using either the Picard or the Newton-Raphson solution algorithm. For one-dimensional cases where convergence difficulties are not expected, the efficiency of these two algorithms has been found to be similar. For certain steady-state cases involving highly nonlinear soil moisture characteristics, the use of the Newton-Raphson algorithm is preferable, particularly when its counterpart fails to converge within a reasonable number of iterations (say between 10 and 20).

3.2.2 Solute Transport

A numerical approximation of the one-dimensional transport equation is obtained using an upstream-weighted finite element formulation with spatial discretization performed using linear elements. Time integration is performed using a central finite difference approximation. This leads to a system of linear algebraic equations. The equation corresponding to node i takes the form:

$$\alpha_i \, c_{i-1}^{k+1} + \beta_i \, c_i^{k+1} + \gamma_i \, c_{i+1}^{k+1} = d_i \qquad (3.5)$$

where α_i, β_i, γ_i, and d_i are given by

$$\alpha_i = \tau\alpha_i^* + \langle\theta R\rangle_{i-1}\,\Delta z_{i-1}/\,(6\Delta t_k) \tag{3.6a}$$

$$\beta_i = \tau\beta_i^* + (\langle\theta R\rangle_i\,\Delta z_i + \langle\theta R\rangle_{i-1}\,\Delta z_{i-1})\,/\,(3\Delta t_k) \tag{3.6b}$$

$$\gamma_i = \tau\gamma_i^* + \langle\theta R\rangle_i\,\Delta z_i\,/\,(6\Delta t_k) \tag{3.6c}$$

$$\begin{aligned} d_i = {} & (\tau-1)\,(\alpha_i^*\,c_{i-1}^k + \beta_i^*\,c_i^k + \gamma_i^*\,c_{i+1}^k) \\ & + \frac{\langle\theta R\rangle_{i-1}}{6\Delta t_k}\,(c_{i-1}^k + 2c_i^k)\,\Delta z_{i-1} \\ & + \frac{\langle\theta R\rangle_i}{6\Delta t_k}\,(c_{i+1}^k + 2c_i^k)\,\Delta z_i \end{aligned} \tag{3.6d}$$

$$\alpha_i^* = -\frac{\langle D\rangle_{i-1}}{\Delta z_{i-1}} - \frac{(1+\omega)}{2}\langle V\rangle_{i-1} + \frac{\lambda\langle\theta R\rangle_{i-1}\,\Delta z_{i-1}}{6} \tag{3.6e}$$

$$\begin{aligned} \beta_i^* = {} & \left[\frac{\langle D\rangle_{i-1}}{\Delta z_{i-1}} + \frac{\langle D\rangle_i}{\Delta z_i}\right] + \frac{\lambda}{3}\left(\langle\theta R\rangle_{i-1}\,\Delta z_{i-1} + \langle\theta R\rangle_i\,\Delta z_i\right) \\ & + \frac{(1+\omega)}{2}\langle V\rangle_{i-1} - \frac{(1+\omega)}{2}\langle V\rangle_i \end{aligned} \tag{3.6f}$$

$$\gamma_i^* = -\frac{\langle D\rangle_i}{\Delta z_i} + \frac{(1+\omega)}{2}\langle V\rangle_i + \frac{\lambda\langle\theta R\rangle_i\,\Delta z_i}{6} \tag{3.6g}$$

with τ and ω denoting the time weighting factor and the upstream weighting factor, respectively.

To obtain a second-order temporal approximation, the value of τ is set equal to 1/2. This corresponds to using the Crank-Nicolson central difference time stepping scheme. The upstream weighting factor ω is introduced in the above numerical approximation to curb numerical oscillations that may occur when the selected finite element grid is not sufficiently refined for a given value of longitudinal dispersivity. For each time step, the linear system of algebraic equations is solved using the Thomas algorithm.

In designing a finite element grid for transport simulations, one should select nodal spacings that will yield reasonable approximations to the expected concentration distributions. The selection of nodal spacing (Δz) and time step value (Δt) should follow the so-called Peclet number and Courant number criteria where possible. These two criteria are given as follows:

$$\frac{\Delta z}{\alpha_L} \leq 4 \tag{3.7}$$

$$V_{sol}\, \Delta t/\Delta z \leq 1 \tag{3.8}$$

$$V_{sol} = V/(\theta R) \tag{3.9}$$

where α_L is the longitudinal dispersivity, and V_{sol} is the solute velocity, V = Darcy velocity, θ = water content, and R = retardation coefficient.

The SAMFT1D code also provides the user with the option of using upstream weighting to curb numerical oscillations that may occur in solving the advective-dispersive transport equation. The recommended value of ω is determined by using the following formulas:

$$\omega = 1 - 4\alpha_L/\ell \quad , \quad \ell > 4\alpha_L$$
$$\omega = 0 \quad , \quad \ell \leq 2\alpha_L$$

where α_L is the longitudinal dispersivity, and ℓ is the length of the element.

3.3 NUMERICAL TREATMENT OF MULTIPHASE FLOW PROBLEMS

3.3.1 Three-Phase Flow System

3.3.1.1 Numerical Formulation of Flow Equations

The fully implicit finite difference scheme is used to discretized Eqs. (2.15) - (2.17), in terms of the three primary variables, P_n, S_w and S_n. The resulting non-linear algebraic equations are solved by the Newton-Raphson method. A block-centered grid is used for the spatial discretization, as shown in Figure 3.2.

The following difference operators are used:

$$\Delta X \Delta Y = X_{i+1/2} (Y_{i+1} - Y_i) + X_{i-1/2} (Y_{i-1} - Y_i) \tag{3.10}$$

for a second order finite difference approximation to:

$$\frac{\partial}{\partial z} \left[X \frac{\partial}{\partial z} Y \right] \tag{3.11}$$

for the time difference:

$$\Delta^t P = P^{n+1} - P^n \tag{3.12}$$

and for the iteration:

$$\delta P = P^{k+1} - P^{k} \tag{3.13}$$

where subscript i represents grids for space discretization, superscript n is the time level, at which all the variables are known, and superscript k is used to denote iteration levels.

At grid i, multiplying Eq. (2.15) - (2.17) by (A Δz_i), discretizing the resulting equations, and moving all terms in the right-hand side into the left-hand side, we have the following set of three completed non-linear algebraic equations in a residual form:

$$R_\ell(x_{\beta,j}) = [\Delta T_\ell \Delta \Phi_\ell\ ]^{n+1} + Q_\ell^{n+1} - \frac{V_i}{\Delta t}\Delta^t\ (\phi \rho_\ell S_\ell) = 0 \tag{3.14}$$

where

Q_ℓ = $V_i q'_\ell\ \rho_\ell$, mass source/sink term in node i (M/T)

V_i = A Δz_i, volume of node i (L^3)

β = primary variable index, β=1, 2, and 3

j = grid index, j = i-1, i, and i+1

$x_{\beta,j}$ = primary variables, $x_{1,j} = S_{w,j}$, $x_{2,j} = S_{n,j}$, and $x_{3,j} = P_{n,j}$, at node j

A = cross-sectional area (L^2)

and the finite difference operator is defined as:

$$\Delta T_\ell \Delta \Phi_\ell = T_{\ell,i+1/2}\ (\Phi_{\ell,i+1} - \Phi_{\ell,i}) + T_{\ell,i-1/2}\ (\Phi_{\ell,i-1} - \Phi_{\ell,i}) \tag{3.15}$$

The potential function for phase ℓ at node i is defined as:

$$\Phi_{\ell,i} = P_{\ell,i} - \rho_\ell g z_i \tag{3.16}$$

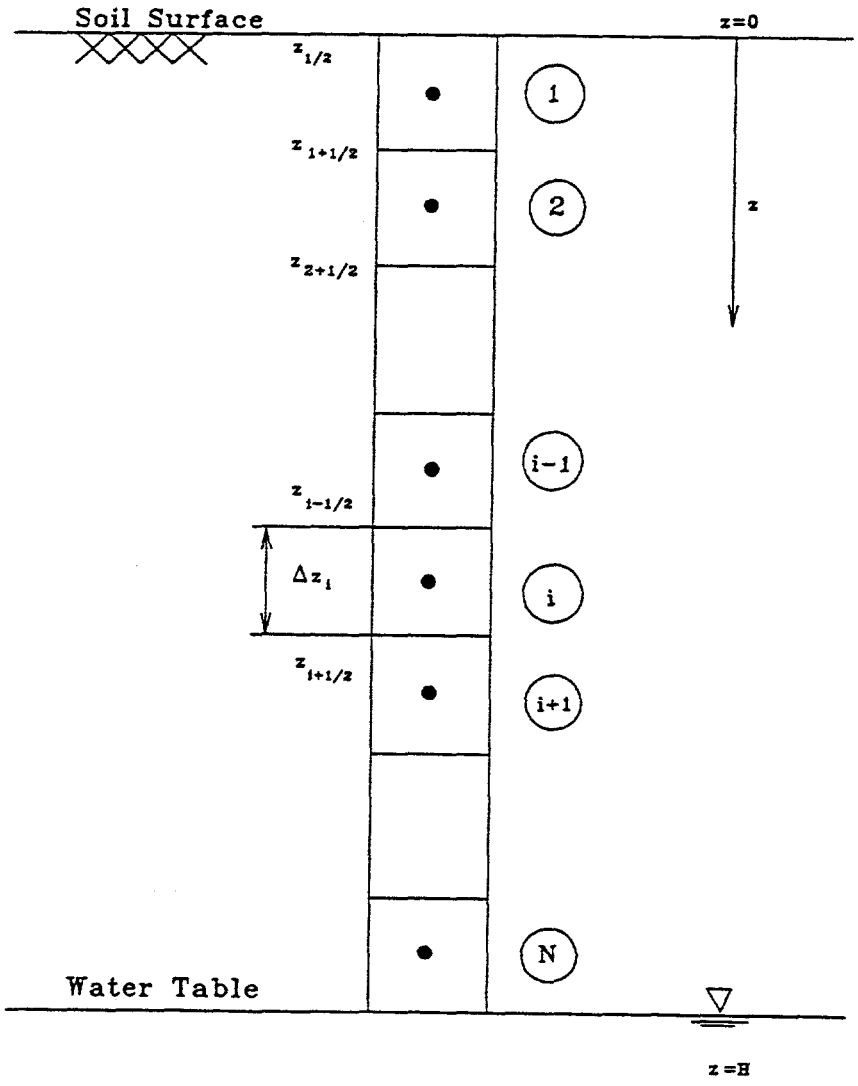

Figure 3.2 Block-centered finite difference discretization of soil column showing grids and coordinates.

and the transmibility between node i and node i+1,

$$T_{\ell,i+1/2} = \frac{\kappa_{i+1/2}}{\mu_\ell} (\rho_\ell k_{r\ell})_{i+1/2} \tag{3.17}$$

with

$$\kappa_{i+1/2} = \frac{2\ A\ k_i\ k_{i+1}}{k_{i+1}\ \Delta z_i + k_i\ \Delta z_{i+1}}$$

Eq. (3.14) can be linearized for variables at iteration step k+1 in terms of the primary variables at iteration k,

$$\begin{aligned} R_\ell^{k+1}(x_{\beta,j}) = R_\ell^k(x_{\beta,j}) &+ \frac{\partial R_\ell^{k+1}}{\partial S_w}\Big|_k\ \delta S_w \\ &+ \frac{\partial R_\ell^{k+1}}{\partial S_n}\Big|_k\ \delta S_n + \frac{\partial R_\ell^{k+1}}{\partial P_w}\Big|_k\ \delta P_w = 0 \end{aligned} \tag{3.18}$$

where

$$R_\ell^k(x_{\beta,j}) = (\Delta T_\ell \Delta\Phi_\ell)^k + Q_\ell^k - \frac{V_i}{\Delta t}\left\{(\phi\rho_\ell S_\ell)^k - (\phi\rho_\ell S_\ell)^n\right\} \tag{3.19}$$

For each element (grid block) with volume V_i there are three equations for the three phase mass conservation, so that for a flow system with N grid blocks Eq. (3.18) represents a set of 3 x N linear equations for the unknown increments δS_w, δS_n, and δP_n.

Eq. (3.18) can be further written in a matrix form as

$$[A]\ \vec{X} = \vec{B} \tag{3.20}$$

where the Jacobian **[A]** is a block tridiagonal matrix, defined as

$$\mathbf{[A]} = \begin{bmatrix} J_{1,1} & J_{1,2} & & & \\ J_{2,1} & J_{2,2} & J_{2,3} & & \\ \ddots & \ddots & \ddots & & \\ & J_{i,i-1} & J_{i,i} & J_{i,i+1} & \\ & \ddots & \ddots & \ddots & \\ & & J_{N,N-1} & J_{N,N} & \end{bmatrix} \tag{3.21}$$

with the submatrix components:

$$J_{i,j} = \begin{bmatrix} \frac{\partial R_w^i}{\partial S_{w,j}} & \frac{\partial R_w^i}{\partial S_{n,j}} & \frac{\partial R_w^i}{\partial P_{n,j}} \\ \frac{\partial R_n^i}{\partial S_{w,j}} & \frac{\partial R_n^i}{\partial S_{n,j}} & \frac{\partial R_n^i}{\partial P_{n,j}} \\ \frac{\partial R_a^i}{\partial S_{w,j}} & \frac{\partial R_a^i}{\partial S_{n,j}} & \frac{\partial R_a^i}{\partial P_{n,j}} \end{bmatrix} \tag{3.22}$$

which consists of the derivatives of R_ℓ (ℓ=w, n, and a) at node i (i = 1, 2, ..., N) with respect to the primary variables, S_w, S_n, and P_n at node j (j = i-1, i, and i+1); the increment vector of the primary variables $\vec{X}$ is defined as:

$$\vec{X} = (\vec{X}_1, \vec{X}_2, \ldots, \vec{X}_N)^T \tag{3.23}$$

with the components defined as

$$\vec{X}_i = (\delta S_{w,i},\ \delta S_{n,i},\ \delta P_{n,i})^T \qquad (i = 1, 2, \ldots, N) \tag{3.24}$$

The right-hand side term in Eq. (3.20) is

$$\vec{B} = (\vec{R}_1, \vec{R}_2, \ldots, \vec{R}_N)^T \tag{3.25}$$

with

$$\vec{R}_i = - (R_w^k, R_n^k, R_a^k)^T \tag{3.26}$$

where R_ℓ^k (ℓ = w, n and a) defined by Eq. (3.19).

All the derivatives $\frac{\partial R_\ell}{\partial S_w}$, $\frac{\partial R_\ell}{\partial S_n}$, and $\frac{\partial R_\ell}{\partial P_n}$ in the Jacobian matrix (3.21) or (3.22) are evaluated by numerical differentiation, i.e., the derivatives at node i with respect to changes of primary variables, S_w, S_n, and P_n, at node j (j = i-1, i, i+1) are determined by

$$\frac{\partial R_\ell^i}{\partial x_{\beta,j}} = \frac{R_\ell^k (x_{\beta,j} + \epsilon_\beta) - R_\ell^k (x_{\beta,j})}{\epsilon_\beta} \tag{3.27}$$

where ϵ_β are increments of S_w, S_n, and P_n, for β = 1, 2, and 3, respectively, to calculate the numerical derivatives.

Since Eqs. (3.14) are mass balance equations, the flow terms between nodes i-1 and i, and i and i+1 will not change at iteration k. Thus, Eq. (3.27) can be simplified and the off-diagonal terms in the Jacobian matrix in Eq. (3.21) can be calculated by

$$\frac{\partial R_\ell^i}{\partial x_{\beta,j}} = \frac{F_{\ell,ij}\,(x_{\beta,j} + \epsilon_\beta) - F_{\ell,ij}\,(x_{\beta,j})}{\epsilon_\beta} \tag{3.28}$$

where the mass flow terms $F_{\ell,ij}$ of phase ℓ between nodes i and j (j = i-1, or i+1) is given by

$$F_{\ell,ij}\,(x_{\beta,j}) = \frac{\kappa_{i\pm1/2}}{\mu_\ell}\,(\rho_\ell k_{r\ell})^{ups}\,(\Phi_{\ell,j} - \Phi_{\ell,i}) \tag{3.29}$$

in which the fully upstream weighting technique is used to evaluate the relative permeability terms (Forsyth, 1990):

$$(\rho_\ell k_{r\ell})^{ups} = (\rho_\ell k_{r\ell})_j \qquad if \qquad (\Phi_{\ell,j} > \Phi_{\ell,i}) \tag{3.30}$$

and

$$(\rho_\ell k_{r\ell})^{ups} = (\rho_\ell k_{r\ell})_i \qquad if \qquad (\Phi_{\ell,j} \le \Phi_{\ell,i}) \tag{3.31}$$

Only for the diagonal terms (j=i) do we need to consider the source/sink and accumulation terms in Eq. (3.27):

$$\begin{aligned}\frac{\partial R_\ell^i}{\partial x_{\beta,i}} = \Big[& F_{\ell,ii-1}\,(x_{\beta,_i} + \epsilon_\beta) + F_{\ell,ii+1}\,(x_{\beta,i} + \epsilon_\beta) \\ & - M_\ell\,(x_{\beta,i} + \epsilon_\beta) + Q_\ell(x_{\beta,i} + \epsilon_\beta) - R_\ell^k(x_{\beta,i}) \Big]\end{aligned} \tag{3.32}$$

where the accumulation terms M_ℓ are defined as

$$M_\ell(x_{\beta,i}) = \frac{V_i}{\Delta t}\left[(\phi\rho_\ell S_\ell)^k - (\phi\rho_\ell S_\ell)^n\right] \tag{3.33}$$

and the treatment of source/sink terms Q_ℓ for the boundary conditions will be discussed in the next section.

After the Jacobian coefficients in Eq. (3.22) for each grid are calculated before next iteration at each time step, the 3×N linear algebraic equations (3.20) will be solved using a block tri-diagonal matrix solver (Panday and Corapcioglu, 1991). Iteration is continued until the relative or absolute errors of the primary variables are reduced below a preset convergence tolerance.

3.3.1.2 Treatment of Boundary Conditions

All types of boundary conditions in the multiphase flow modules of the code SAMFT1D are treated fully implicitly in terms of source or sink terms. At the top boundary, z=0, if the mass flux of phase ℓ is specified by Eq. (2.55) the mass source terms used in Eq. (3.20) are calculated by:

$$Q_{\ell,1} = q_\ell^o \qquad (\ell = w,\ n,\ and\ a) \tag{3.34}$$

where subscript 1 denotes node 1. When only one injection pressure P_β^o of phase β (β = w, n, or a) is specified on the surface, Eq. (2.54), then the mass source terms for phase ℓ (ℓ = w, n, and a) at the first node are given by (Fanchi et al., 1982):

$$Q_{\ell,1} = - PI_1 \rho_\ell \left[P_\ell - P_\beta^o + \frac{\Delta z_1}{2} \rho_\ell g \right] \sum_{\ell=1}^{3} \left[\frac{k_{r\ell}}{\mu_\ell} \right] \tag{3.35}$$

where

$$PI_1 = \frac{2Ak_1}{\Delta z_1} \tag{3.36}$$

and the total mobility is used (Thomas, 1982). Since, for most application problems, only one phase pressure needs to be specified for injection, the code treats the source terms for phases whose pressure is not prescribed on the boundary as follows:

$$Q_{\ell,1} = 0 \quad (\ell \neq \beta) \tag{3.37}$$

if $Q_{\ell,1} > 0$, given by (3.35), such that the only injected fluid is that whose pressure is described at the boundary.

If the number of specified pressures is equal to that of active phases on the top boundary, the code will calculate the mass source terms for each fluid also using Eq. (3.35) with $\beta = \ell$, and force the constraint,

$$Q_{\ell,1} \geq 0 \quad (\ell = w, n, \textit{and } a) \tag{3.38}$$

so that no fluid is allowed to produce (exit) from node 1.

The bottom boundary for node i = N is treated as sink or outflow boundary in the code. Either flux or pressure conditions can be prescribed. If a total liquid production rate q_T^B from the last node, Eq. (2.57), is prescribed, a bottom boundary pressure P_B is first calculated as:

$$P_B = \frac{-|q_T^B| + PI_N \sum_{\ell=1}^{2} \frac{\rho_\ell k_{r\ell}}{\mu_\ell} \left(P_\ell + \frac{\Delta z_N}{2} \rho_\ell g\right)}{PI_N \sum_{\ell=1}^{2} \frac{\rho_\ell k_{r\ell}}{\mu_\ell}} \tag{3.39}$$

with

$$PI_N = \frac{2Ak_N}{\Delta z_N} \tag{3.40}$$

If $P_B < P_{atm}$, i.e., the boundary pressure calculated from (3.39) is smaller than atmospheric pressure, it implies that the target rate q_T^B cannot be achieved, and then the code will set,

$$P_B = P_{atm} \tag{3.41}$$

to calculate actual fluxes. For either case whether $P_B \geq P_{atm}$, or $P_B < P_{atm}$ from Eq. (3.39), the mass sink term for phase ℓ is given by:

$$Q_{\ell,N} = -PI_N \frac{k_{r\ell}\rho_\ell}{\mu_\ell} \left[P_\ell - P_B + \frac{\Delta z_N}{2} \rho_\ell g\right] \tag{3.42}$$

$$(\ell = w, n \text{ and } a)$$

If a pressure is prescribed on the bottom boundary by Eq. (2.56), the mass source/sink terms are generated by the code as:

$$Q_{\ell,N} = - PI_N \frac{k_{r\ell}\rho_\ell}{\mu_\ell} (P_\ell - P_B + \frac{\Delta z_N}{2} \rho_\ell g) \quad (3.43)$$

The mass fluxes across the bottom boundary calculated from (3.43) are subject to the following constraints:

$$Q_{\ell,N} \leq 0 \qquad \text{for } \ell = \text{n, a} \quad (3.44)$$

i.e., NAPL or air can only flow out of the bottom boundary, and water can flow either into or out of the boundary node. It should be mentioned that the source/sink equations discussed above be evaluated using the primary variables of the boundary nodes.

3.3.1.3 Treatment of Default Initial Conditions

In a multiphase flow simulation, the undisturbed initial condition of the system is considered to be at equilibrium between capillary pressure and gravity in SAMFT1D. The code provides three options for initialization of default initial conditions for three primary variables, S_w, S_n, and P_n, based on the assumption that the initial saturation (S_{no}) of the second fluid phase (NAPL) and the initial pressure (P_{atm}), of the third phase (air) are constants. The equations used in the code to calculate the undefined initial conditions of the primary variables are as follows:

$$S_n(z,0) = S_{no}(z) \quad (3.45a)$$

and

$$P_a(z,0) = P_{atm} \quad (3.45b)$$

Since the initial state of the system may be under two-phase (water and air) or three-phase (water, NAPL and air) conditions, a generalized capillary pressure function, (2.30), is used to relate liquid phase saturation to the difference in phase pressures,

$$P_{cal}(S_w, S_a) = \hat{\alpha}\left[P_{can}(S_a) + P_{cnw}(S_w)\right] + (1 - \hat{\alpha})\, P_{caw}(S_a) \tag{3.46}$$

where

$$P_{cal} \overset{def.}{=} \bar{P}_{can} + \bar{P}_{cnw} = P_a - P_w$$

(i) If initial water pressure P_w is prescribed, the equation:

$$P_{atm} - P_w(z_i, 0) = P_{cal}\left[S_{wo}, 1 - S_{wo} - S_{no}(z_i)\right] \quad (i = 1, 2, \ldots, N) \tag{3.47}$$

is used to determine the initial water saturation $S_{wo} = S_w(z_i, o)$. Then NAPL pressures are calculated by

$$P_n(z_i, 0) = P_w(z_i, 0) + \hat{\alpha}\, P_{cnw}(S_{wo}) + (1 - \hat{\alpha})\, P_{cnw}(S_w = 1) \quad (i = 1, 2, \ldots, N) \tag{3.48}$$

(ii) If water potential Φ_w ($\Phi_w = P_w - \rho_w gz$) is described, the code will convert the potential profile to a water pressure profile by

$$P_w(z_i, 0) = \Phi_w(z_i) + \rho_w^o g z_i$$
$$(i = 1, 2, \ldots, N)$$

Then, water saturation and NAPL pressure distributions are computed using Eq. (3.47) and (3.48), respectively.

(iii) If the default initial primary variable is water saturation S_{wo},

$$S_w(z,0) = S_{wo}(z) \tag{3.50}$$

the water pressure is determined by

$$P_w(z_i,0) = P_{atm} - \hat{\alpha}\left[P_{cnw}(S_{wo}(z_i)) + P_{can}\left[1 - (S_{wo}(z_i) + S_{no}(z_i))\right]\right] \tag{3.51}$$
$$(i = 1, 2, \ldots, N)$$

Then NAPL pressure is calculated by Eq. (3.48).

3.3.2 Two-Phase Flow in a Three-Phase System

3.3.2.1 Numerical Formulation of Flow Equations

The governing equations for two-phase (water and NAPL) flow in a three-phase (water, NAPL and air) system can be derived from the three-phase flow equations (2.15)-(2.17). The air pressure is assumed to be constant, and the air conservation equation (2.17) is therefore eliminated. Consequently, the liquid saturation can be obtained from the air-NAPL capillary pressure relation. The primary variables of the numerical solution in this case are NAPL pressure P_n and saturation S_n. The total five unknowns, P_w, P_n, S_w, S_n and S_a can be solved from equations (2.15), (2.16), (2.22), (2.23), and (2.24). The constitutive relations for relative permeability should be evaluated exactly as in three-phase flow situations.

The finite difference scheme and numerical formulation used for two-phase flow in a three-phase system are almost identical to those discussed in Section 3.3.1 for the three-phase flow case except that the fluid phase index ℓ ranges from 1(w) to 2(n) instead of 1(w), 2(n), and 3(a) for the three-phase flow. The final linearized algebraic equations of 2×N for the primary variables P_n and S_n for a one-dimensional flow system with N block-centered grids are given in the same form as in Eq. (3.20). However, the submatrices in the Jacobian [A] in Eq. (3.20) are replaced by 2×2 matrices for node i,

$$J_{i,j} = \begin{bmatrix} \frac{\partial R_w^i}{\partial P_{n,j}} & \frac{\partial R_w^i}{\partial S_{n,j}} \\ \frac{\partial R_n^i}{\partial P_{n,j}} & \frac{\partial R_n^i}{\partial S_{n,j}} \end{bmatrix} \tag{3.52}$$

instead of 3×3 matrices by Eq. (3.22) and the subvectors in $\bar{X}$ and $\bar{B}$ have only two elements. The coefficients of derivatives of Eq. (3.52) are also calculated by Eqs. (3.28) and (3.32) with $\ell = 1, 2$ and $\beta = 1, 2$ only.

3.3.2.2 Treatment of Boundary Conditions

The treatment of boundary conditions for the two-phase flow version in a three-phase system of SAMFT1D is the same as that for the three-phase flow discussed in Section 3.3.1. Pressure or flux specified boundary conditions are treated fully implicitly as sink/source terms for the two phases at the first and the last nodes, which can be implemented by setting ℓ = w and n instead of ℓ = w, n, and a in the sink/source equations in Section 3.3.1.

3.3.2.3 Treatment of Default Initial Conditions

The code provides three options to generate the initial conditions for two-phase (water and air) flow in a three-phase system, which are the same as in the three-phase flow case, discussed in Section 3.3.1.3.

3.3.3 Two-Phase Flow in a Two-Phase System

3.3.3.1 Numerical Formulation of Flow Equations

The governing equations for only two-phase (water and NAPL) flow problems can be derived simply by dropping the air equation (2.17), using Eqs. (2.15) and (2.16) only. The fluid index reduces to two, ℓ = w and n, the constraint condition for saturation now becomes,

$$S_w + S_n = 1 \tag{3.53}$$

The constitutive equations are also simplified by taking off all the relationships for air phase. The capillary pressure is given by Eq. (2.25) or (2.28), and the relative permeability is by Eq. (2.31) and

$$k_{rn} = k_{rn}(S_w) \tag{3.54}$$

as a function of water saturation only.

The primary variables for the two-phase case are selected as NAPL pressure P_n and saturation S_n, so water pressure and saturation are expressed in terms of P_n and S_n by Eq. (2.23) and

$$S_w = 1 - S_n \tag{3.55}$$

Initial conditions should be specified as in Eqs. (2.51) and (2.53), and boundary conditions are such as Eqs. (2.54) - (2.57) with ℓ = w and n only.

The finite difference scheme and numerical formulation used for two-phase flow is almost identical to those discussed in Section 3.3.2 for the two-phase flow case in a three-phase system. The final linearized algebraic equations of 2×N for the primary variables P_n and S_n at a one-dimensional flow system with N block-centered grids are given in the same form as in Eqs. (3.52) and (3.20).

3.3.3.2 Treatment of Boundary Conditions

The treatment for the two-phase flow version of SAMFT1D are the same as that two-phase flow in a three-phase system as discussed in Section 3.3.1.

3.3.3.3 Treatment of Default Initial Conditions

The code provides two options to generate the initial conditions for two-phase (water and NAPL) flow, assuming that the initial saturation of NAPL phase is known as

$$S_n(z,\ 0) = S_{no}(z) \tag{3.56}$$

A generalized capillary curve (2.28) between water and NAPL phases is used to correlate the phase pressures,

$$\bar{P}_{cnw}(S_w) = \hat{\alpha} P_{cnw}(S_w) + (1 - \hat{\alpha}) P_{cnw}(S_w = 1)$$

(i) For initial water pressure P_w profiles prescribed, NAPL pressure is calculated from:

$$P_n(z_i, 0) = P_w(z_i, 0) + \bar{P}_{cnw}(1 - S_{no}(z_i)) \quad (i = 1, 2, \ldots, N) \tag{3.57}$$

(ii) For initial water potential Φ_w profiles described, NAPL pressure is calculated from:

$$P_n(z, 0) = \Phi_w(z_i) + \rho_w^o g z_i + \bar{P}_{cnw}\,(1 - S_{no}(z_i)) \tag{3.58}$$

The two primary variables, P_n and S_n, are then determined.

3.3.4 Nonlinear Iteration and Time Stepping Schemes

In treating a nonlinear multiphase flow problem, iterations must be performed within each time step to obtain a converged numerical solution. During each iteration, nodal values of the unknown variables need to be updated for the next iteration. Furthermore, time step adjustments need to be made to handle convergence problem and to obtain an efficient transient simulation. Therefore, the iterative Newton-Raphson scheme is used in the multiphase flow modules of SAMFT1D to solve the nonlinear finite difference equations (3.14). Convergence is considered to be achieved if the following criteria are satisfied:

$$max \left| \frac{\delta x_{\beta,i}}{x_{\beta,i}} \right| \leq \epsilon_{r\beta} \quad (\beta=1,2, \textit{ and } 3;\ i=1,2,\ldots,N) \tag{3.59}$$

for relative convergence tolerance specified, or

$$\max \mid \delta x_{\beta,i} \mid \leq \epsilon_{a\beta} \ , \ (\beta=1,2, \ and \ 3; \ i=1,2,\ldots,N) \tag{3.60}$$

for absolute convergence tolerance specified, where $\delta x_{\beta,i}$ are changes in primary variables $x_{\beta,i}$ at node i over an iteration, $\epsilon_{r\beta}$ and $\epsilon_{a\beta}$ are input relative and absolute convergence tolerances for x_{β}, respectively.

3.3.4.1 Automatic Under-Relaxation Scheme

The updating of the nodal values of the unknown variables is performed using an automatically determined under-relaxation factor and a scheme dependent upon the maximum convergence errors for the entire mesh. The following relaxation formula is used to obtain improved estimates of the nodal unknowns:

$$x_{\beta,i}^{k+1} = x_{\beta,i}^{k} + \Omega^{k+1} \delta \, x_{\beta,i}^{k+1} \tag{3.61}$$

where k+1 and k denote current and previous iterations, respectively, and Ω^{k+1} is a relaxation factor for the current iteration. The value of Ω^{k+1} is determined from:

$$\Omega^{k+1} = \min \left\{ \frac{S^*}{\max|\delta S_{\beta,i}|}, \frac{P^*}{\max|\delta P_{n,i}|}, 1 \right\} \tag{3.62}$$

$$(\beta = 1, 2, \ and \ 3; \ i = 1, 2, \ldots, N)$$

subject to

$$0.1 \leq \Omega^{k+1} \leq 1.0 \tag{3.63}$$

where S^* is a parameter related to maximum changes in saturation allowed over an iteration (approximately 0.1 ~ 0.2); P^* is a parameter related to maximum changes in pressure allowed over an iteration (approximately 1 bar).

3.3.4.2 Determination of Computational Time Step Size

Computational time steps for the transient flow simulation are determined using the following procedures:

(i) The first time step Δt_1 needs to be input, then SAMFT1D automatically updates the value of the following time steps, Δt_n, (n = 2, 3, ...) depending on how quickly the solution converged at the previous time step. If satisfactory convergence was obtained, determine the subsequent computational time steps using the following algorithm used by Forsyth (1990):

$$\Delta t_{n+1} = \min (TFAC * \Delta t_n, \Delta t_{max}) \quad (n = 1, 2, \ldots) \tag{3.64}$$

for $k \leq k_{max}$, where TFAC is determined by

$$TFAC = \min \left\{ \frac{S'}{\max|\Delta^t S_{\beta,i}|}, \frac{P'}{\max|\Delta^t P_{n,i}|} \right\} \quad (\beta = 1, 2, \textit{and } 3; \textit{ and } i = 1, 2, \ldots, N) \tag{3.65}$$

subject to

$$0.001 \leq TFAC \leq 5 \tag{3.66}$$

where TFAC is a multiplication factor, Δt_{max} is maximum time step allowed, and k_{max} is maximum number of iterations allowed per time step, S′ is a parameter related to maximum changes in saturation allowed over a time step (approximately 0.1 ~ 0.2), and P′ is a parameter related to maximum changes in pressure allowed over a time step (approximately 1 bar).

(ii) If convergence difficulty was encountered (i.e. solution fails to converge within the allowable maximum number of nonlinear iterations, k_{max}), then reduce the computational time step size according to the following scheme:

$$\Delta t_{n+1} = \Delta t_n / TDIV \tag{3.67}$$

where TDIV is the time step divider set equal to 2, 5 and 10 for n = 1,2, and greater or equal to 3, respectively.

(iii) If necessary, adjust the computational time step, Δt_n, to obtain t_{n+1} value that coincides with a target time value at which simulation output is required.

3.4 NUMERICAL TREATMENT OF MULTIPHASE SOLUTE TRANSPORT PROBLEMS

The multiphase transport of a single contaminant component was developed in Chapter 2 and the governing equation was given as (2.59). The equation contains extra terms describing the fate of precipitated mass in addition to the standard advection-dispersion-reaction terms. Since the development of the finite element equations for the usual solute transport part is well known and can be found in any text books (see for example Huyakorn and Pinder, 1983), only a brief description is given in this section for standard procedures. However, a detailed derivation will be offered for non-standard features.

In the finite element solution technique, the continuum solutions c and m (in which the subscripts w and p are removed for the sake of simplification) are replaced by approximate solutions which are written in terms of interpolation functions. Standard linear interpolation functions are used for both c and m in this study. When the approximate solutions are substituted, the equation (2.59) can not be satisfied. However, the error in the approximate solutions is minimized using the weighted residual method. In this study the upstream weighted residual method (Huyakorn and Pinder, 1983) is employed. The weighted residual equation for an element, after the dispersion term is integrated by parts, becomes

$$\left[\phi R_T\left(\frac{dc_j}{dt} + \lambda c_j\right) + \left(\frac{dm_j}{dt} + \lambda m_j\right)\right]\int_{x_-^e}^{x_+^e} N_i N_j\, dx$$
$$= -\left[D_T\int_{x_-^e}^{x_+^e}\frac{\partial N_j}{\partial x}\frac{\partial W_i}{\partial x}\,dx + V_T\int_{x_-^e}^{x_+^e} W_i\frac{\partial N_j}{\partial x}\,dx\right]c_j + D_T\frac{\partial c}{\partial x}W_i\Big|_{x_-^e}^{x_+^e} \qquad (3.68)$$

where the element is defined by $x\epsilon[x_-^e, x_+^e]$. The interpolation and the weighting functions are

$$\begin{aligned} N_1 &= 1 - \xi \\ N_2 &= \xi \\ W_1 &= 1 - \xi + 3\alpha(\xi^2 - \xi) \\ W_2 &= \xi - 3\alpha(\xi^2 - \xi) \end{aligned}$$

in which $\xi = (x - x_-^e)/(x_+^e - x_-^e)$ and $\alpha\epsilon[0,1]$ controls the amount of upwinding and is specified by the user. Full upstream weighting is obtained when $\alpha = 1$. Upwinding can be used to suppress numerical oscillations, but care must be taken in interpreting results since the solution, although smooth, contains artificial dispersion.

Note that in deriving (3.68) all the physical parameters, except for c and m, are assumed to be piecewise constant within an element. The semi-discrete equation (3.68) is further discretized in time using the variable weight θ in the usual manner:

$$\left(\frac{\Delta x \phi \bar{R}_T}{\Delta t}\int_0^1 N_i N_j d\xi + \theta \Omega_{ij}\right) c_j^{k+1} + \left(\frac{\Delta x}{\Delta t} + \theta \Delta x \lambda\right)\int_0^1 N_i N_j d\xi \; m_j^{k+1}$$

$$= \left(\frac{\Delta x \phi \bar{R}_T}{\Delta t}\int_0^1 N_i N_j d\xi + (\theta - 1)\Omega_{ij}\right) c_j^{k} + \left(\frac{\Delta x}{\Delta t} + (\theta - 1)\Delta x \lambda\right)\int_0^1 N_i N_j d\xi \; m_j^{k}$$

$$+ \theta \bar{D}_T \left(\frac{\partial c}{\partial x}\right)^{k+1} W_i \Big|_0^{\Delta x} - (\theta - 1)\, \bar{D}_T \left(\frac{\partial c}{\partial x}\right)^{k} W_i \Big|_0^{\Delta x} \qquad (3.69)$$

where $\Delta x = x_+^e - x_-^e$, $\Delta t = t^{k+1} - t^k$, and

$$\Omega_{ij} = \Delta x \phi \bar{R}_T \lambda \int_0^1 N_i N_j d\xi + \bar{V}_T \int_0^1 W_i \frac{\partial N_j}{\partial \xi}\, d\xi$$

$$+ \frac{\bar{D}_T}{\Delta x}\int_0^1 \frac{\partial W_i}{\partial \xi}\frac{\partial N_j}{\partial \xi}\, d\xi$$

in which a barred variable indicates that the initially time dependent variable was simplified to be time independent during the time step. The representative value for any variable for the time step is obtained by

$$\bar{x} = \theta x^{k+1} + (1 - \theta) x^k$$

The time discretization scheme becomes the Crank-Nicholson and the fully implicit schemes when θ assumes the value of 1/2 and 1, respectively.

The global finite element equations are obtained by assembling all individual finite element equations for all elements. Then, the following system of linear equations results:

$$A_{ij}\, c_j^{k+1} + B_{ij}\, m_j^{k+1} = D_{ij}\, c_j^{k} + E_{ij}\, m_j^{k} + f_i \qquad (3.70)$$

where the tridiagonal matrices A, B, D and E contains all physical and geometrical information, and the vector f contains the boundary condition information.

At this point it is important to point out one weakness in (3.70). While the continuum equation (2.59) indicates that the dependence of the precipitated mass on the spatial variable is implicit, the finite element interpolation function gives an explicit dependence. The explicit dependence results in the non-diagonal coefficient matrices B and E, and sometimes causes temporal oscillations in the concentration profile at a neighboring node. The explicit dependence can be removed by lumping the consistent mass matrices B and E through the usual row sum method. Numerical experiments indicate that the temporal oscillations due to the explicit dependence can be successfully removed using the lumped matrices. It can also be shown rigorously that the resulting discretized equations using the lumped mass matrices are closer to the differential equation than the discretized equations resulting from the consistent matrices.

The solution of the tridiagonal matrix equation can be obtained very efficiently. However, the equation (3.70) appears to have two unknowns at each node, but c and m are mutually exclusive and there always is only one unknown at each node at one time. The equation (3.70) can be reorganized so that only unknowns at the time level k+1 appear on the left hand side. Then,

$$H_{ij}\, u_j^{k+1} = -K_{ij}\, v_j^{k+1} + D_{ij}\, c_j^{k} + E_{ij}\, m_j^{k} + f_i \qquad (3.71)$$

where the vectors u and v are combinations of c and m, and contain only unknown and known variables at the time level k+1 and k, respectively. The matrices H and K are obtained from

A and B by combining appropriate columns. Once the solution to the equation (3.71) is obtained, the constraint relations (2.75) and (2.76) are examined. If the constraints are satisfied at all nodes, the solution proceeds to the next time step. However, if any of the two constraints is violated at a node, the other variable, previously considered to be known, becomes unknown and the coefficient matrices H and K are modified by exchanging the appropriate columns. The new tri-diagonal system of equations is solved again for the correct variables.

It is important to note that the variable switching will be enforced even when the violation of constraints is due to numerical oscillations.

3.5 NUMERICAL TREATMENT OF CAPILLARY HYSTERESIS EFFECTS

The constitutive relation of fluid saturation against capillary pressure for fluids in porous media typically exhibits hysteresis. The relationship is not a single-valued function, but depends on the imbibition-drainage history of the fluid in the medium. This leads to a multitude of possible p-S curves, bounded by the envelope described by the main drainage $S^d(p)$ curve and main imbibition $S^i(p)$ curve. A procedure is described below which enables arbitrary scanning curves in the S(p) relation to be computed given the boundary curves, $S^i(p)$ and $S^d(p)$, and the fluid saturation history of the system. Only slight modifications are required to evaluate hysteretic p(S) relationships, i.e., when saturations rather than pressures are used as primary variables. The proposed procedure satisfies the physical requirement that intermediate scanning loops be closed.

A typical hysteretic S(p) relation is shown in Figure 3.3 and will be referred to illustrate the calculation procedure. The figure shows the main drainage, $S^d(p)$, and the main imbibition,

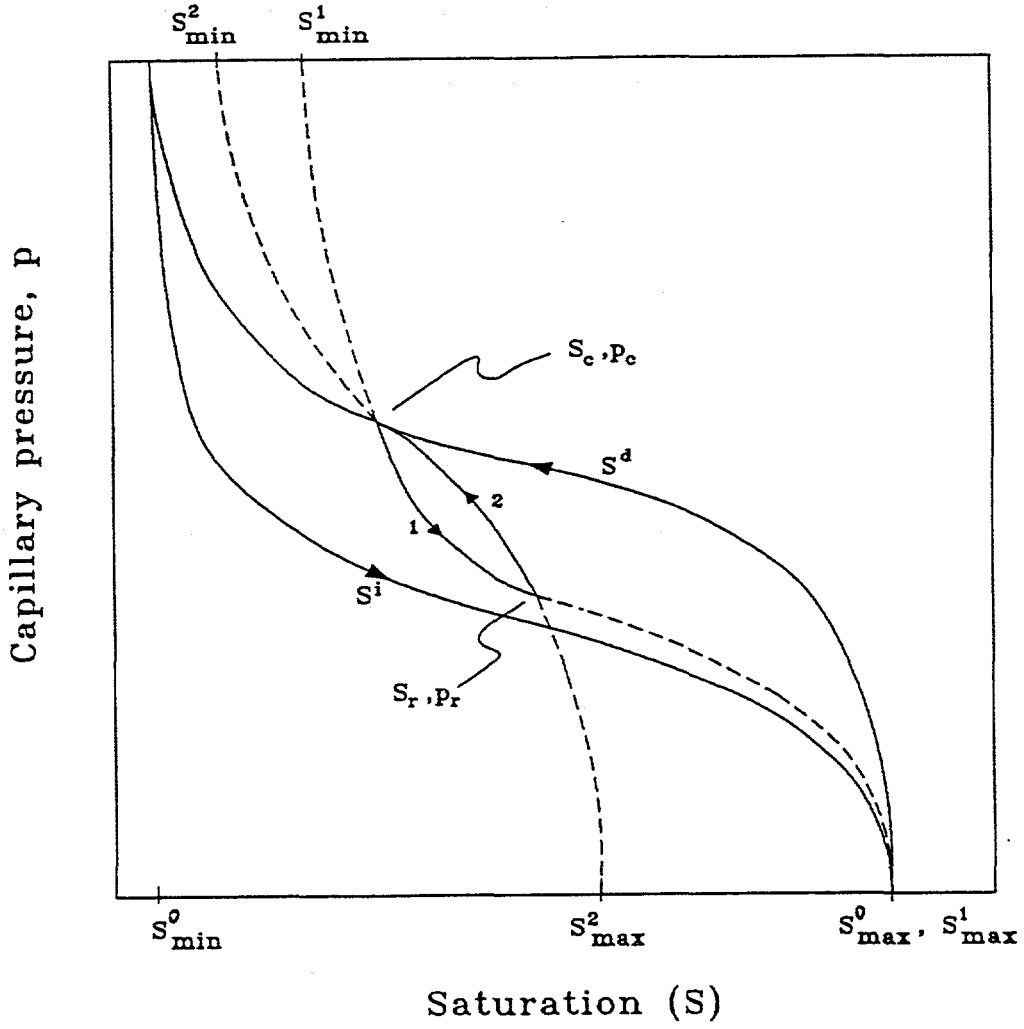

Figure 3.3. Typical hysteretic saturation - capillary pressure relation.

$S^w(p)$, curves as well as a primary imbibition scanning curve, $S^1(p)$, and a secondary drainage scanning curve, $S^2(p)$. The two scanning curves form a closed loop, bounded by the points [S_r, p_r] and [S_c, p_c]. The point [S_r, p_r] is the reversal point on the scanning loop from imbibition to drainage; the point [S_c, p_c] represents the closure point of the scanning loop.

Saturation values on the main imbibition and the drainage curves are bounded by S^0_{max} and S^0_{min} (Note: saturations may be scaled such that $S^0_{max} = 1$ and $S^0_{min} = 0$, however this does not need to be the case). The boundary S(p) curves are described by

$$S^d(p) = S^0_{min} + (S^0_{max} - S^0_{min})\, F^d(p) \tag{3.72}$$

$$S^i(p) = S^0_{min} + (S^0_{max} - S^0_{min})\, F^i(p) \tag{3.73}$$

and where F^d and F^i are the soil characteristic functions with $0 \leq F \leq 1$. Typical characteristic functions are proposed by van Genuchten (1980):

$$F^d(p) = \left[1 + (\alpha^d p)^{\beta^d}\right]^{-\gamma^d} \tag{3.74}$$

and

$$F^i(p) = \left[1 + (\alpha^i p)^{\beta^i}\right]^{-\gamma^i} \tag{3.75}$$

with

$$\gamma = 1 - 1/\beta$$

The procedure for evaluating saturations on the scanning curves $S^1(p)$ and $S^2(p)$ is based on a rescaling of the boundary imbibition and drainage curves, such that

$$S^1(p) = S^1_{min} + (S^1_{max} - S^1_{min})\ F^i(p) \tag{3.76}$$

and

$$S^2(p) = S^2_{min} + (S^2_{max} - S^2_{min})\ F^d(p) \tag{3.77}$$

The parameters S^1_{min}, S^1_{max}, S^2_{min}, and S^2_{max} are the scaling parameters which are determined in such a way that closure of the scanning loop is enforced. For the present example it may be noted that since S^1 represents a primary imbibition scanning curve (originating from the main drainage curve), the parameter S^1_{max} is given by $S^1_{max} = S_{max}$. Conversely, for all primary drainage curves the value of S^1_{min} is given by $S^1_{min} = S_{min}$.

The procedure for evaluating S(p) is illustrated by going through the calculation for a point located on the drainage scanning curve $S^2(p)$. Saturation values on this scanning curve are given by:

$$S(p) = S^2_{min} + (S^2_{max} - S^2_{min})\ F^d(p) \tag{3.78}$$

where S^2_{max} and S^2_{min} are as yet unknown coefficients. They are determined by requiring that the scanning curve passes through the two points:

$$S(p_r) = S_r = S^2_{min} + (S^2_{max} - S^2_{min})\ F^d(p_r) \tag{3.79}$$

and

$$S(p_c) = S_c = S^2_{min} + (S_{max} - S^2_{min})\ F^d(p_c) \tag{3.80}$$

Equation (3.79) can be rewritten as

$$S_{max} - S_{min} = \frac{S_r - S_{min}}{F(p_r)} \tag{3.81}$$

where superscripts have been dropped to simplify notation. Next, (3.81) is substituted in (3.80) which yields

$$\begin{aligned} S_c &= S_{min} + \frac{S_r - S_{min}}{F(p_r)} F(p_c) \\ &= S_{min} + S_r \frac{F(p_c)}{F(p_r)} - S_{min} \frac{F(p_c)}{F(p_r)} \end{aligned} \tag{3.82}$$

Rearrangement of Eq (3.82) yields for S_{min}

$$S_{min} = \left[S_c - \frac{F(p_c)}{(Fp_r)} \right] \left[1 - \frac{F(p_c)}{F(p_r)} \right]^{-1} \tag{3.83}$$

With S_{min} obtained from (3.83), the coefficient S_{max} is calculated directly from (3.81).

The procedure for calculating imbibition scanning curves is the same as outlined above, except that $F^i()$ is used instead of $F^d()$. This procedure can be used for any order scanning curve. The required information is thus as follows: (1) whether the current saturation state is a imbibition or a drainage condition; (2) the saturation, S_r, and capillary pressure, p_r, at the most recent reversal in saturation state; (3) the values of S_c and p_c at the closure point of the current scanning loop. The latter values are the same as the reversal saturation and pressure, respectively, at the second-to-last reversal in saturation state. The main imbibition and drainage curves can also be defined in this way. For the main imbibition branch, the reversal and closure

points are given by $[S_r,p_r] = [S^0_{min}, p_{min}]$ and $[S_c, p_c] = [S^0_{max}, p_{max}]$. The corresponding parameters for the main drainage curve are $[S_r, p_r] = [S^0_{max}, p_{max}]$ and $[S_c, p_c] = [S^0_{min}, p_{min}]$. When the closure point of a scanning loop is reached, e.g., the point $[S_c, p_c]$ for the secondary drainage curve $S^2(p)$ in example shown in Figure 3.3, the current scanning curve is abandoned and the S(p) relation is given again by the main branch or lower order scanning curve that was being followed when the just completed scanning loop was initiated. For the example of Figure 3.3, this means that upon continued drainage, the main drainage boundary $S^d(p)$ is followed.

Implementation of (3.72) - (3.83) in a numerical flow simulation model is straight forward. In addition, some bookkeeping is required in order to obtain an operational computational routine depending on the formulation of the numerical scheme. The following information is required, either for every node or every grid block:

(1) The order of the present scanning curve, i.e., 0,1,2...etc. When a reversal occurs, the scanning curve order is incremented by 1. When a closure point is reached, the scanning curve order is decremented by 2.

(2) Values of the reversal points for the present and all lower order scanning curves. This information is required to determine the appropriate scanning loop closure point when a reversal in the saturation path occurs.

(3) Values of the coefficients S_{min} and S_{max} for the present scanning curve. The values are computed every time when a reversal or scanning loop closure occurs.

The check for reversal and adjustment of the various coefficients are typically made at the end of each time step, and are performed for every node (element) in the computational domain. The updated values are then used during the next simulation time step. Theoretically, the order

of a scanning curve can become infinitely large and the computer storage requirements for satisfying (2) above would be correspondingly large. In practice, therefore, the highest order of a scanning curve considered is 3 or 4; beyond this, hysteresis is ignored.

The procedure outlined above is generic in nature and does not depend on any specific fluid. In multiphase flow systems, the same procedure is followed for each fluid phase. The same approach can be used also when fluid saturations, rather than pressures are used as primary simulation variables. Interchanging saturations and pressures, the pressure-saturation relationship (3.72) is written as

$$p(S) = \frac{S - S_{\min}}{S_{\max} - S_{\min}} \mathscr{F}(S) \tag{3.84}$$

where $\mathscr{F}(\cdot) = F^{-1}(\cdot)$ is the inverse of the adopted soil characteristic curve. For instance, using the van Genuchten (1980) relation, we have

$$\mathscr{F}(S) = \frac{1}{\alpha}\left[S^{-1/\gamma} - 1\right]^{1/\beta} \tag{3.85}$$

The procedure for updating S_{min} and S_{max} does not change.

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4 VERIFICATION TESTS AND RESULTS

4.1 GENERAL

Four sets of test problems were used for verification of numerical schemes and demonstration of major capabilities of the SAMFT1D code. The first two sets of problems pertain to single-phase variably saturated flow and transport. These problems are as follows:

- Horizontal flow in a soil slab
- Infiltration in a root zone
- Steady infiltration in the unsaturated zone beneath a land disposal unit
- Transient drainage and infiltration in a soil column with hysteresis
- Horizontal transport in a soil slab
- Vertical transport in a root zone
- Vertical transport in a soil column.

The third and fourth sets of problems pertain to multiphase flow and solute transport. These problems are as follows:

- Horizontal two-phase flow without capillary effect
- Vertical two-phase flow without capillary effect
- Horizontal two-phase flow with capillary effect
- Horizontal two-phase imbibition with capillary effect
- Vertical two-phase flow in a three-phase system
- Vertical three-phase flow
- Vertical three-phase with pulse release of NAPL on the surface

- Vertical transport in a soil column
- Vertical transport in a soil column with initial contaminant existing in stagnant NAPL phase.

A detailed description of all test problems, values of the physical parameters used in the simulation, and numerical results are presented in the following sections.

4.2 SINGLE-PHASE FLOW PROBLEMS

4.2.1 Horizontal Flow in a Soil Slab

The purpose of this problem is to test the implementation of the Galerkin finite element formulation and the nonlinear iterative schemes for a one-dimensional case in which there is no gravity effect. The problem, presented in an earlier paper by Huyakorn et al. (1984), is depicted schematically in Figure 4.1. As illustrated, a slab of soil 20 cm long has an initial pressure head of -83.33 cm. Wetting occurs at the left boundary (x = 0) where the pressure head is increased to 0.0 and maintained constant. The pressure head at the right boundary (x = 20 cm) is kept constant at -83.33 cm. For convenience, the soil was assumed to be homogeneous and isotropic with a saturated hydraulic conductivity of 1 cm/d and porosity of 0.45. The soil moisture characteristics used in the simulation are

$$k_{rw} = (S_w - S_{wr})/(1 - S_{wr}) \tag{4.1}$$

and

$$\frac{1-S_w}{1-S_{wr}} = \frac{\psi-\psi_a}{-100-\psi_a} \tag{4.2}$$

where $S_{wr} = 0.3333$ and $\psi_a = 0.0$ cm. The selected relative permeability function corresponds

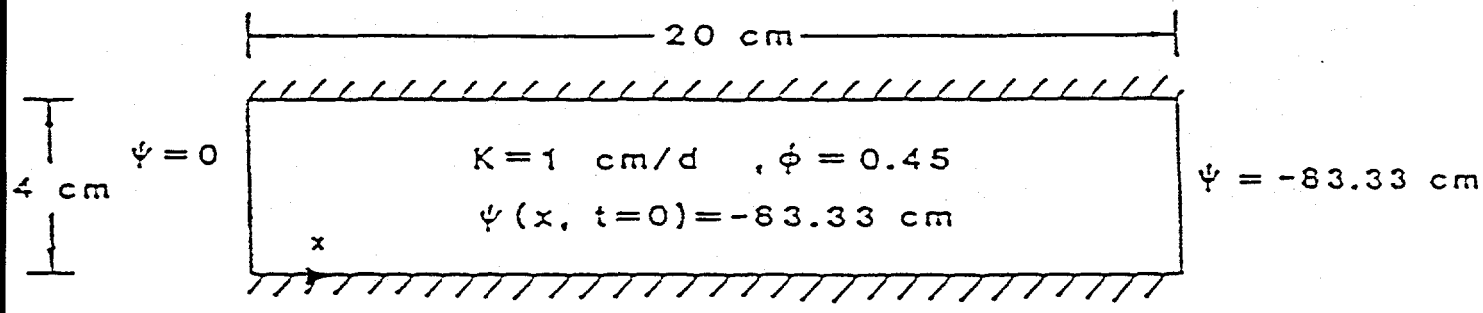


Figure 4.1. Geometry and boundary conditions used in the simulation of unsaturated flow in a soil slab.

to the Brooks-Corey equation with n = 1. The selected water saturation function corresponds to the van Genuchten equation with α = -0.01 cm^{-1}, β = 1 and γ = -1.

To apply the SAMFT1D code to the stated problem, some physical parameters and initial and boundary conditions need to be converted. Table 4.1 provides the result of this conversion. Note that compressibilities of water and soil matrix are assumed to be zero. Numerical solutions were obtained using equal mesh spacings, Δx = 0.25 cm, and constant time increments, Δt = 214 s (.0025 days). Computed water saturation profiles are plotted in Figures 4.2. The saturation values computed by SAMFT1D are compared with the semi-analytical solution of Phillip (1955) and the numerical solution obtained using UNSAT2, the two-dimensional Galerkin finite element code, documented in Neuman et al. (1974) and Davis and Neuman (1983). It can be seen from Figure 4.2 that there is good agreement between the two numerical solutions.

4.2.2 Infiltration in a Root Zone

This problem concerns transient flow in root zone subject to a prescribed amount of infiltration. The problem is depicted in Figure 4.3. The purpose is to demonstrate another application of SAMFT1D to a different type of field problem. The modeled root zone is 100 cm thick and comprised of three layers with contrasting hydraulic properties. The material properties used in the flow simulation are summarized in Table 4.2. Initially, it was assumed that the pressure head distribution in the root zone system was hydrostatic. Transient infiltration was then applied to the top soil for a period of 3 days. The flow simulation was performed for 20 time steps using the Picard scheme with a constant time step value of 0.5 days. Shown in Figures 4.4 and 4.5 are pressure head and water saturation profiles, respectively. The ability

Table 4.1. Converted input parameters and initial and boundary conditions for the SAMFT1D computer run.

Intrinsic permeability, k	1.157E-10	cm^2
Dynamic viscosity of water, μ_w	9.8 E-3	g/(cm.s)
Gravitational acceleration, g	980.5	cm/s^2
Initial gauge pressure value, p_w^o	-81705.1	$dyne/cm^2$
Gauge pressure value at x=0, $p_w(x=0)$	0.0	$dyne/cm^2$
Gauge pressure value at x=20 cm, $p_w(x=20)$	-81705	$dyne/cm^2$

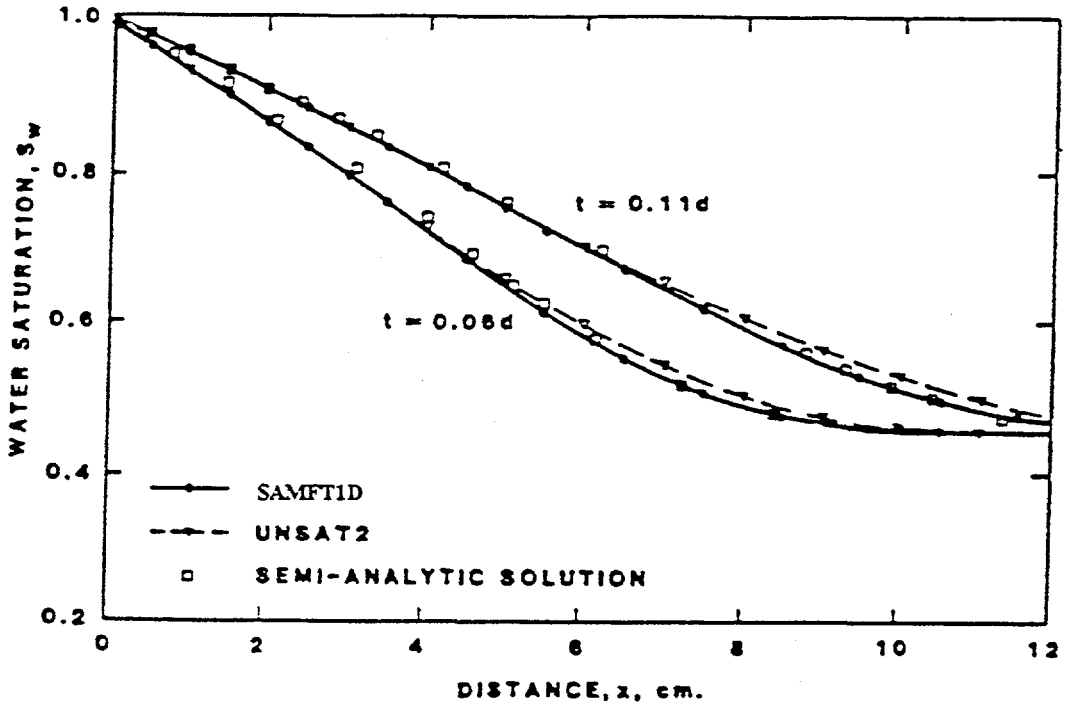


Figure 4.2 Simulated profiles of water saturation during adsorption of water in a soil slab.

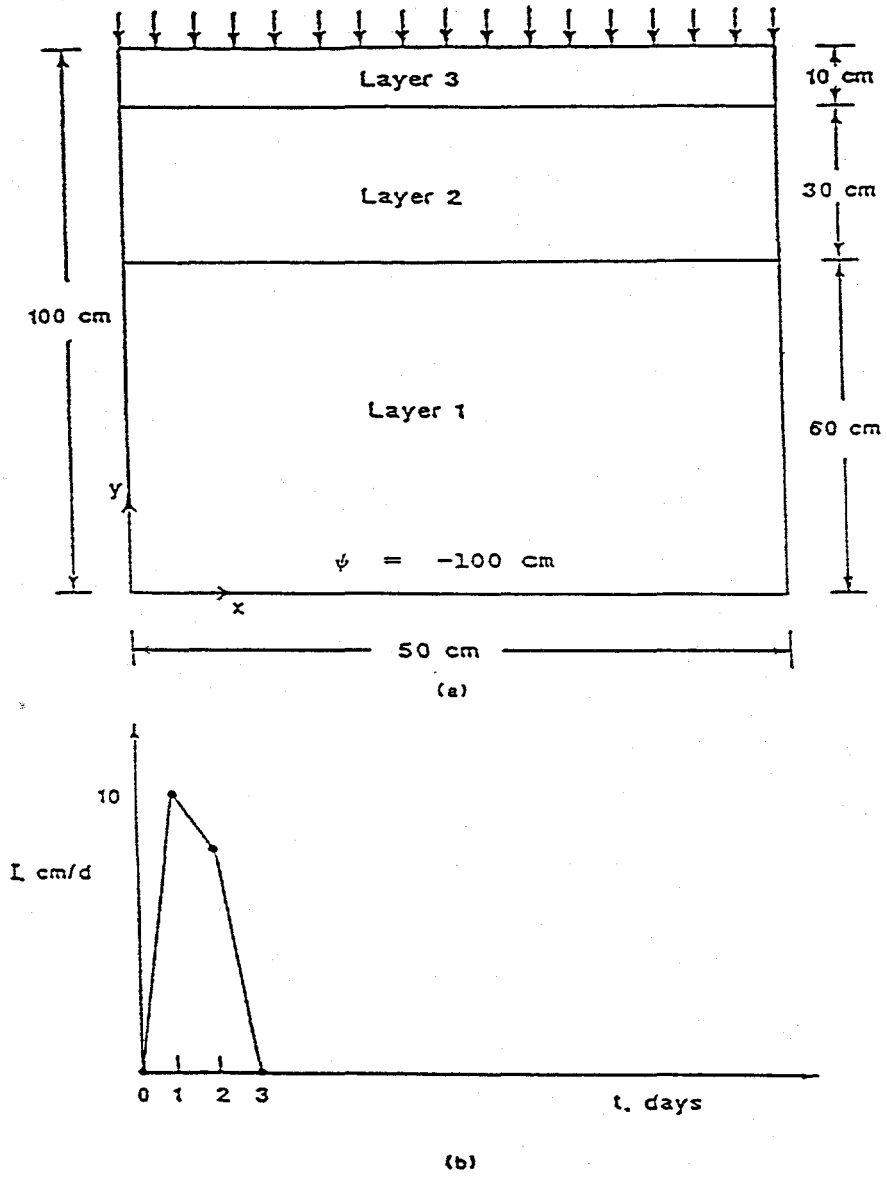


Figure 4.3 Schematic description of the root zone problem.

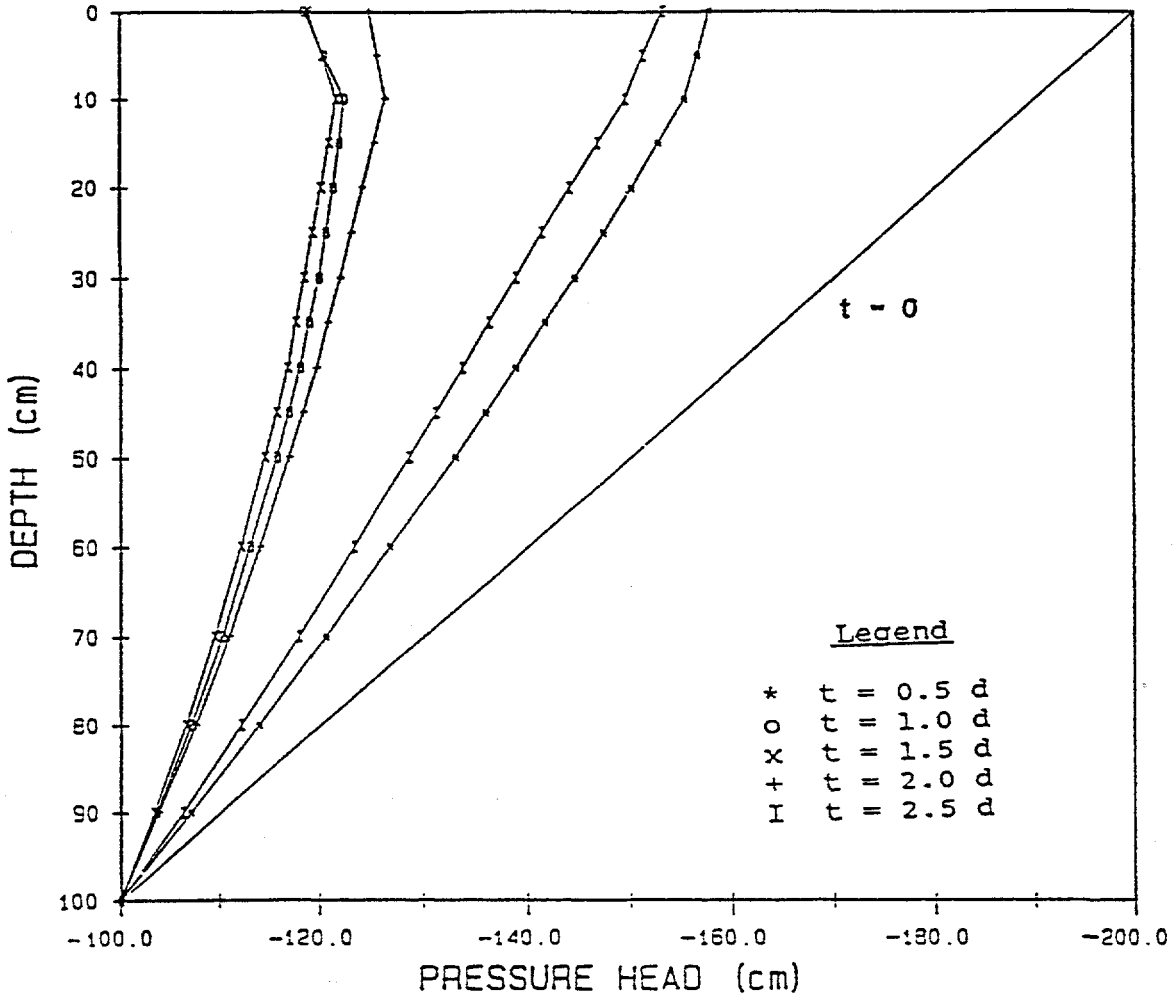


Figure 4.4. Simulated profiles of pressure head in the root zone.

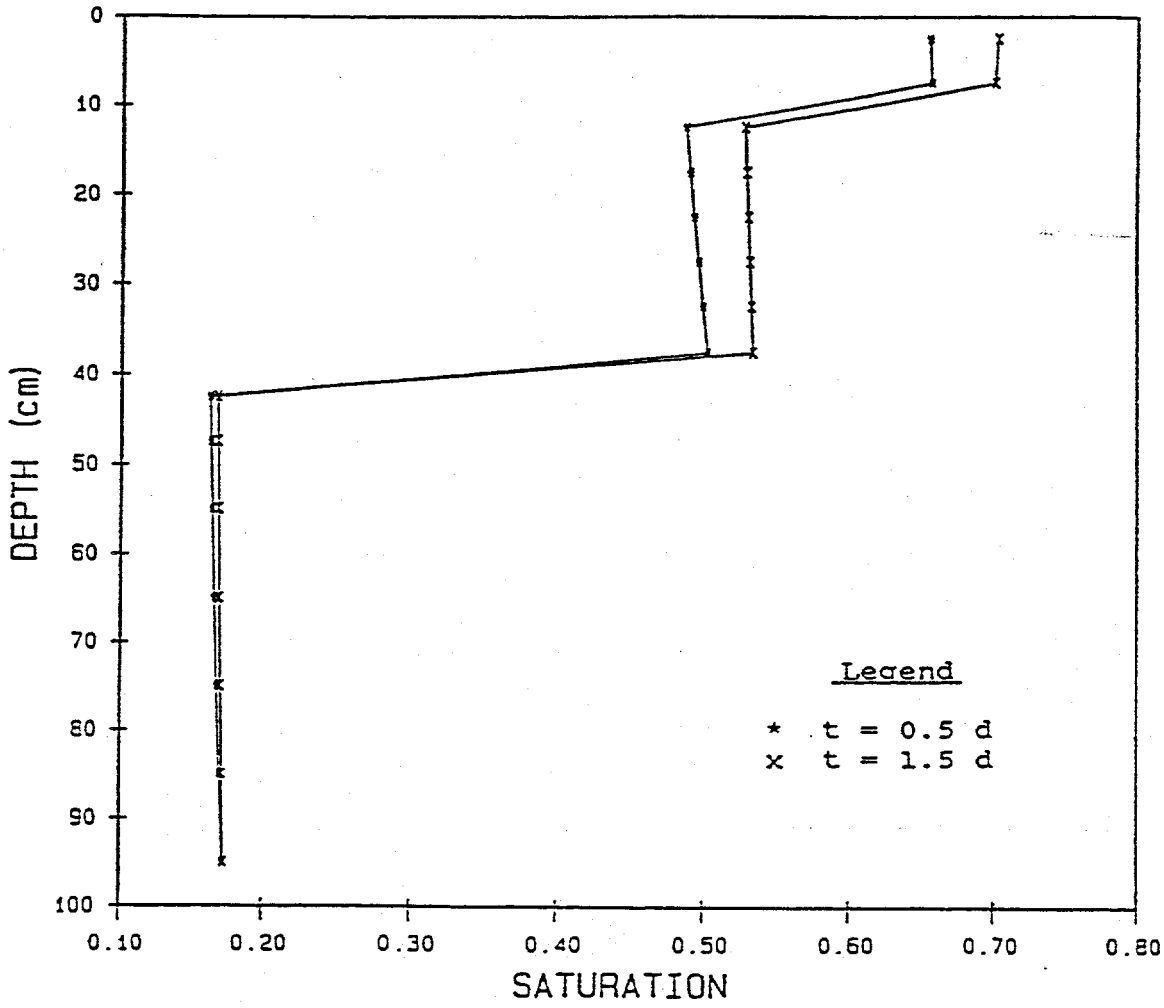


Figure 4.5. Simulated profiles of water-phase saturation in the root zone.

Table 4.2. Material properties used in the simulation of root zone problem.

Layer no.	K, cm/d	k, cm^2	ϕ
1	350	4.05 E-8	0.41
2	25	2.893 E-9	0.43
3	10.8	1.250 E-9	0.45

Layer no.	S_{wr}	n	α cm^{-1}	β
1	0.14	1	0.124	2.28
2	0.18	1	0.036	1.56
3	0.15	1	0.02	1.41

Constitutive relations:

$$k_{rw} = S_e^n$$

$$S_e = 1/[1 + (\alpha \mid \psi \mid)^{\beta}]^{\gamma}$$

where $S_e = (S_w - S_{wr})/(1 - S_{wr})$

of the SAMFT1D code to accommodate rapid response and contrasting properties of the soil system may be noted.

4.2.3 Steady Infiltration in the Unsaturated Zone Beneath a Land Disposal Unit

This problem, solved previously using the VAM2D (Huyakorn et al., 1989) and VADOFT (Huyakorn, et al., 1988) codes, concerns moisture movement and groundwater flow in the unsaturated and saturated zones of an unconfined aquifer system beneath a sanitary landfill. A steady-state analysis of the flow scenario depicted in Figure 4.6 is required before a transient simulation of leachate migration from the landfill can be made. SAMFT1D was used to perform a one-dimensional simulation of flow in the portion of the unsaturated zone that lies directly below the land disposal unit. The constitutive relations used to describe soil moisture characteristics in the vadose zone are as follows:

$$k_{rw} = ((S_w - 0.25)/0.75)^4 \tag{4.3}$$

and

$$(S_w - 0.25)/0.75 = [1 + (0.2\psi)^2]^{-1} \tag{4.4}$$

Note that the soil moisture relations for this particular problem are highly nonlinear. A uniform one-dimensional grid with nodal spacings of 1.75 m was used to represent a soil column beneath the landfill and above the water table. The steady-state simulation was performed in one step (without time marching) using the Newton-Raphson scheme. Satisfactory convergence was achieved in 9 iterations. Shown in Figure 4.7 are simulation results. For the soil column directly below the center of land disposal unit, water saturation profiles computed by the VAM2D finite element code are compared with SAMFT1D. This deviation from the strict one-

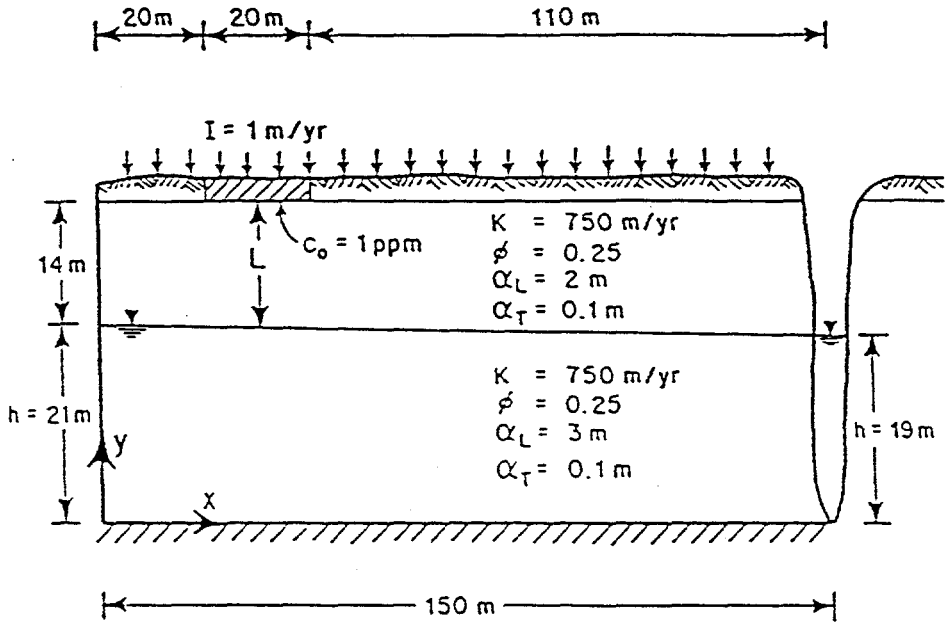


Figure 4.6 Schematic description of the simulated case of water flow in an unsaturated zone beneath a landfill.

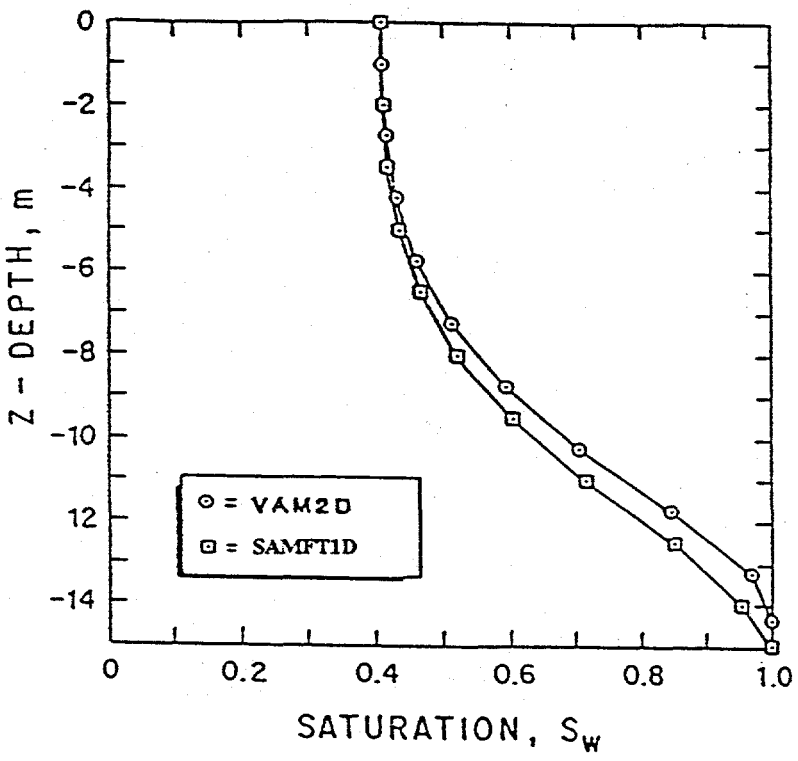


Figure 4.7 Simulated saturation profiles showing comparison of numerical results from SAMFT1D and VAM2D.

dimensional flow assumption used in the SAMFT1D code is likely to be the cause of the difference in the two saturation profiles depicted in the figure.

4.2.4 Transient Drainage and Infiltration in a Soil Column with Hysteresis

This problem involves transient, one-dimensional single-phase flow in a vertical column. The problem simulated is the slow drainage rewet experiment described by Gillham et al. (1979). In this example the soil moisture relationship (Figure 4.8) exhibits considerable hysteresis. The data points in Figure 4.8 represent the experimental data, while the solid lines represent the fitted van Genuchten constitutive curves. The $K(S_w)$ relationship of the material (Dune Sand) is given by the following relationship:

$$K = K_s (S_w)^b$$

Parameter values for the unsaturated flow constitutive relations are given in Table 4.3. The experimental configuration in the experiment of Gillham et al. consisted of an initially saturated, 60 cm tall column. The column was first drained and then rewetted by varying the pressure head at the base of the column. A plot of the controlled bottom boundary pressure head as a function of time is shown in Figure 4.9. The imposed variations in bottom boundary pressure head cause the column to drain (along the boundary drying curve), followed by rewetting (along primary wetting curves) after t = 60 minutes. The SAMFT1D simulation of this experiment is shown in Figure 4.10. The data points in this figure represent measured saturations at t = 68 min and t = 125 min. Saturation profiles predicted by SAMFT1D are represented by the solid lines. The dashed curve represents simulation results obtained using the VAM2D computer

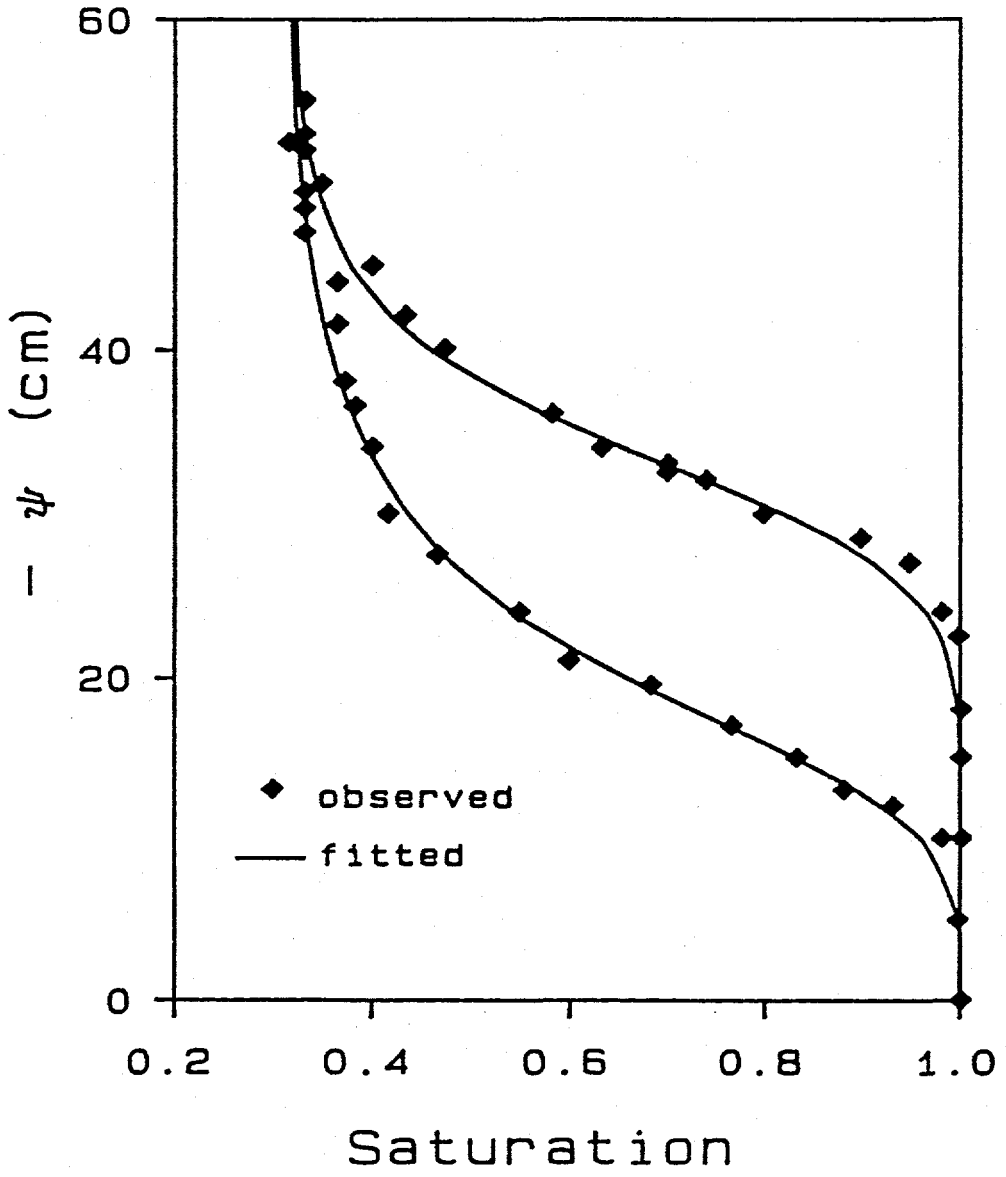


Figure 4.8 Measured hysteretic saturation-pressure head data and fitted van Genuchten curves for Dune sand of problem 4.2.4.

Table 4.3. Parameters for unsaturated flow constitutive relations of Dune Sand.

Parameter	Value
Porosity, ϕ	0.301
Residual saturation, S_{wr}	0.336
Drying curve parameter, α^d	0.0306 cm^{-1}
Wetting curve parameter, α^w	0.0527 cm^{-1}
Curve parameter, β	6.779
Curve parameter, γ	0.852
Saturated conductivity, K_s	23.56 cm/hr
Exponent, b	5.509

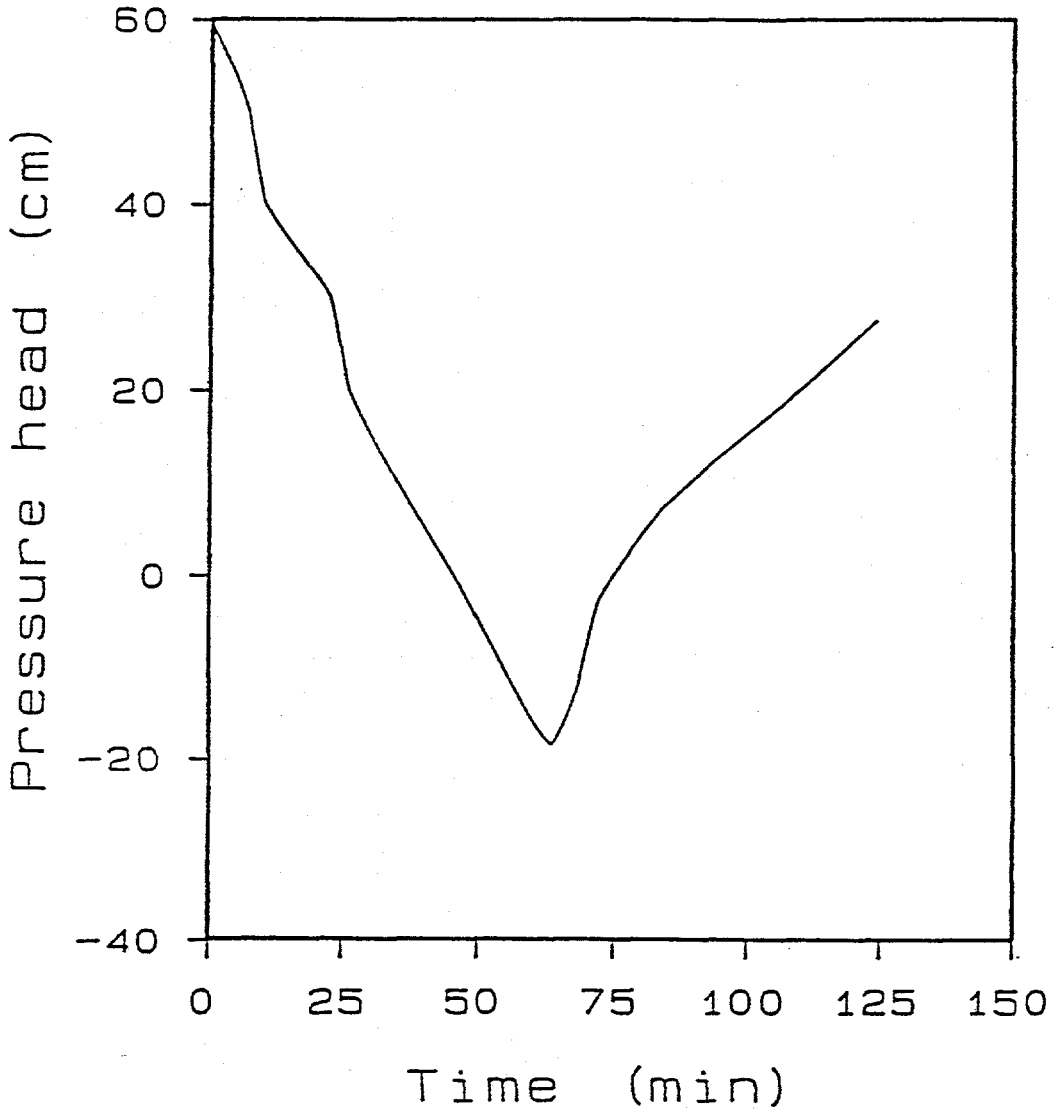


Figure 4.9 A plot of the controlled pressure head at the bottom of the soil column versus time for problem 4.2.4.

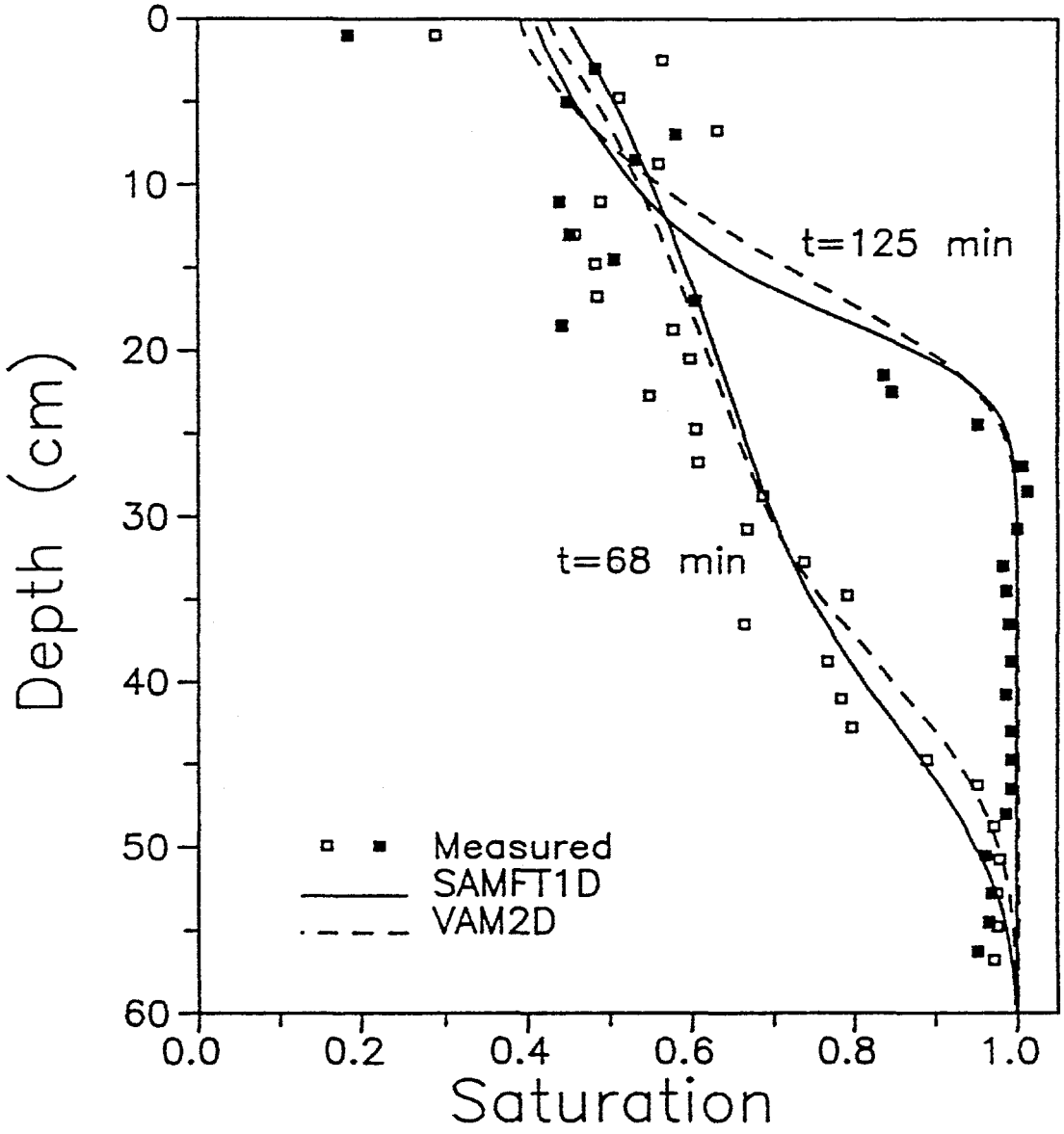


Figure 4.10 Observed and simulated water saturation in soil column for problem 4.2.4. Data points represent measured data; solid and dashed lines represent SAMFT1D and VAM2D results, respectively.

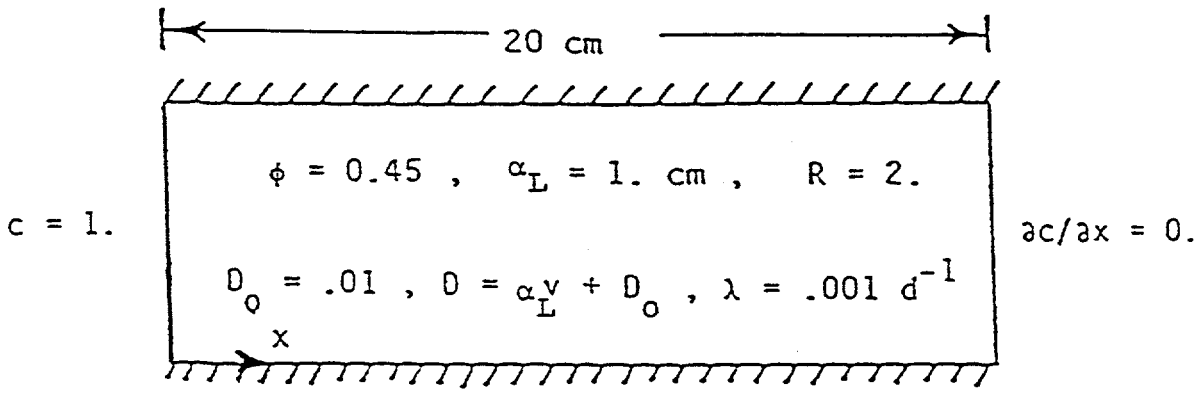
code (Huyakorn et al., 1989). The measured data in Figure 4.10 can be seen to exhibit considerable scatter, especially in the upper part of the column. This was attributed by Gillham et al. to measurement error and lack of homogeneity of the sand material. The SAMFT1D simulation results and those of VAM2D are in generally good agreement with the measured results and with each other. Some deviations between the codes are apparent though. These differences in saturation profiles can be attributed to the somewhat different schemes used in the two codes for computing scanning curves and the use of slightly different parameter values for describing the main wetting and drying curves.

4.3 SINGLE-PHASE TRANSPORT PROBLEMS

4.3.1 Horizontal Transport in a Soil Slab

This problem concerns one-dimensional transport of a non-conservative species in an unsaturated soil slab identical to that described in Section 4.2.1. Velocities obtained by solving the corresponding unsaturated flow problem were used as input data for the current transport problem. Initial and boundary conditions required by the model are depicted in Figure 4.11 together with values of the physical parameters used.

The numerical solution was obtained using a uniform grid with $\Delta x = 0.25$ cm. The problem was run for 50 time steps with a constant value of $\Delta t = 216$ s (.0025 days). Shown in Figure 4.12 is a comparison of SAMFT1D result with those obtained using the semi-analytical solution of Smiles et al. (1978) and the FEMWASTE finite element transport code documented by Yeh and Ward (1981). The numerical and semi-analytical solutions are seen to be in good agreement.



Initial Conditions : c(x,t=0) = 0.

Discretization Data: Δx = 1 cm , Δt = .01 d

Figure 4.11 Schematic description and data for the problem of transport in a soil slab.

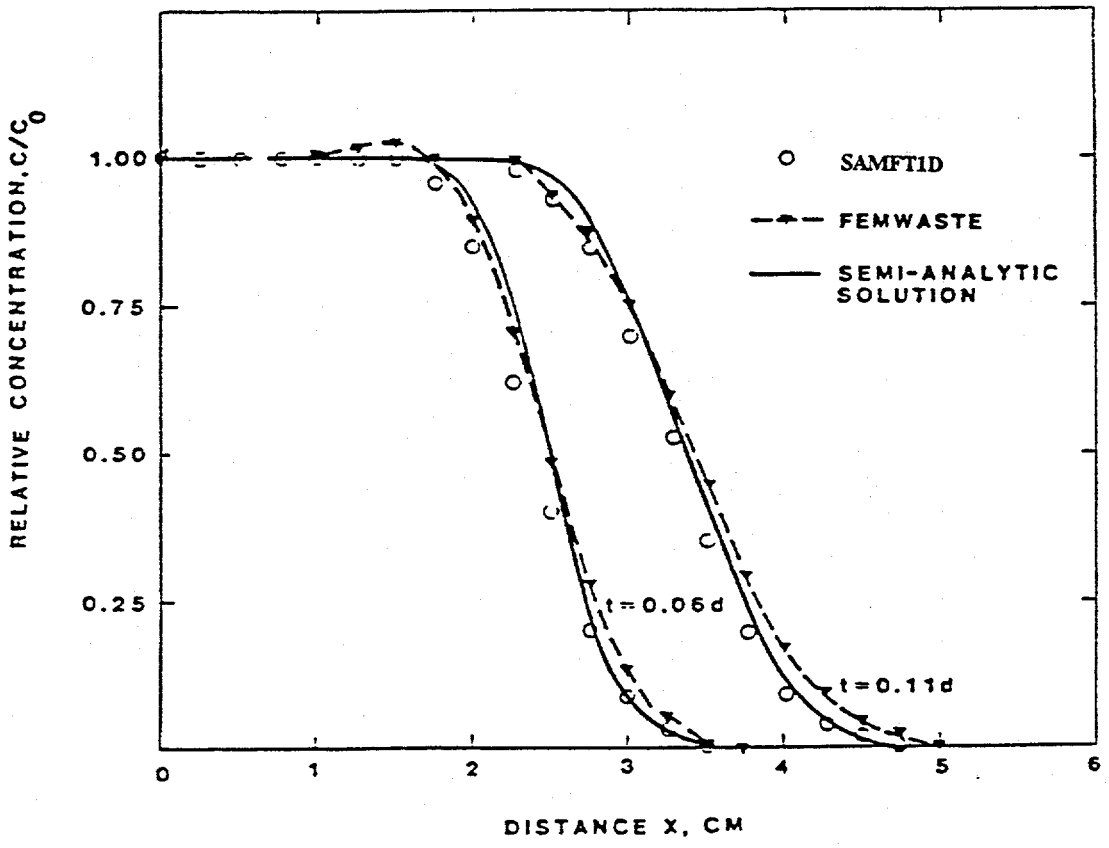


Figure 4.12 Simulated concentration profiles for the problem of one-dimensional solute transport during adsorption of water in a soil tube.

4.3.2 Vertical Transport in a Root Zone

This problem is associated with the flow problem described in Section 4.2.2 and Figure 4.3. Transport of pesticide uniformly applied over the top soil is considered. A first-type boundary condition of unit concentration was assumed at the top surface, and a second type (outflow) boundary condition was assumed at the bottom of the root zone. The transport simulation was performed for 20 time steps using the velocity and water saturation data obtained from the previous flow simulation. Shown in Figure 4.13 is the plot of concentration profiles for five time values. The profiles behave in the manner expected for a layered system.

4.3.3 Vertical Transport in a Soil Column

In this problem, downward vertical transport of dissolved contaminants in a soil column above the water table of an unconfined aquifer is considered. The length of the soil column is 20 m and the Darcy velocity and water content are assumed to be constant and equal to 0.25 m/d and 0.25, respectively. The initial concentration is zero, and water with solute concentration of 1 ppm enters the soil surface at a rate of 0.25 m/d. At the water table, a zero dispersive-flux boundary condition is assumed. A list of physical parameter values and discretization data used in the simulation is provided in Table 4.4. Two cases involving conservative and nonconservative species were simulated. Results obtained from SAMFT1D are compared in Figure 4.14 with the analytical solution given by van Genuchten and Alves (1982). As can be seen, the numerical and analytical solutions for both cases are in excellent agreement.

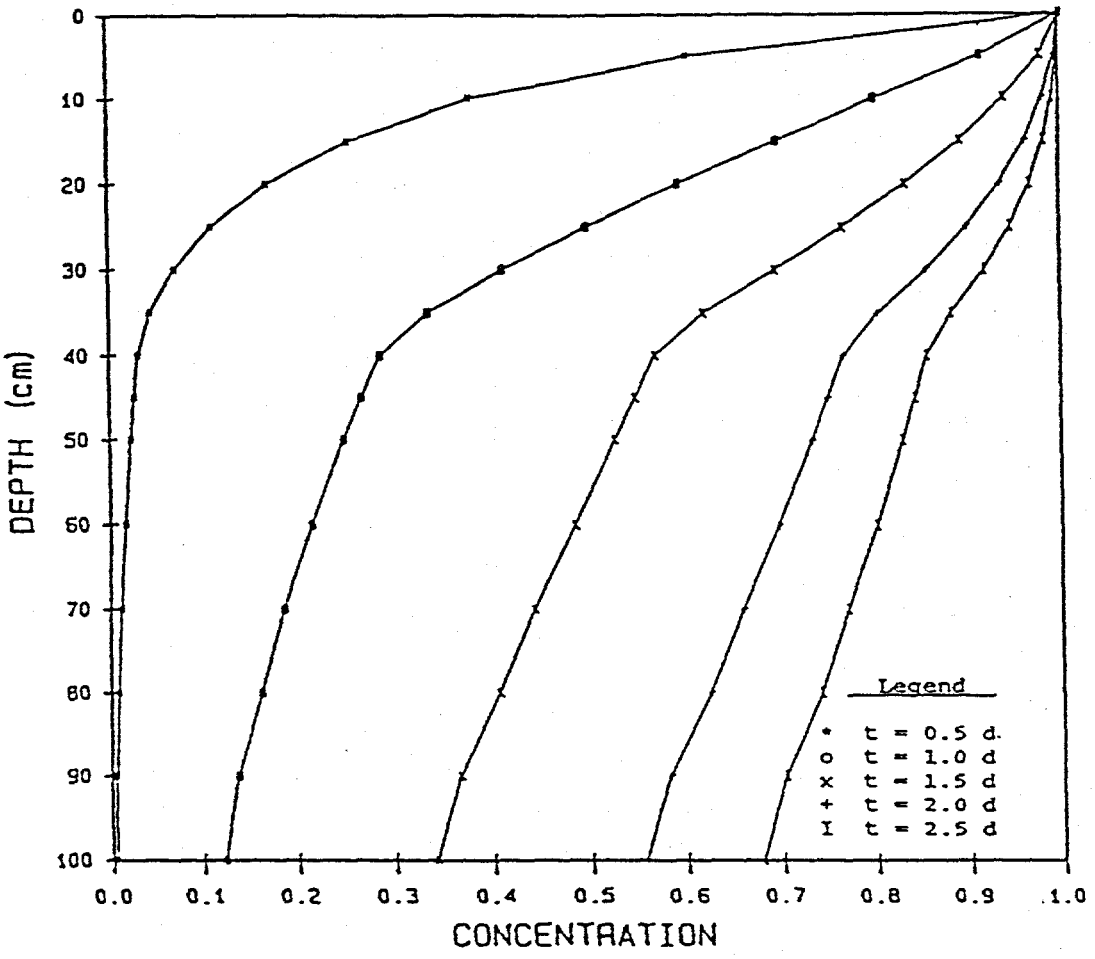


Figure 4.13 Plot of concentration profiles for the root-zone flow and transport problems.

Table 4.4 Values of Physical Parameters and Discretization Data Used in Simulating One-Dimensional Transport in a Finite Soil Column.

PARAMETER	VALUE
Thickness of soil column, L	20 m
Darcy velocity, V	0.25 m/d
Water content, θ	0.25
Retardation coefficient, R	1
Longitudinal dispersivity, α_L	4 m
Source leachate concentration, C_o	1 ppm
<u>Case 1:</u>	
Decay constant, λ	0 d^{-1}
<u>Case 2:</u>	
Decay constant, λ	0.25 d^{-1}
Δz = 1.0 m	
Δt = 0.5 d	

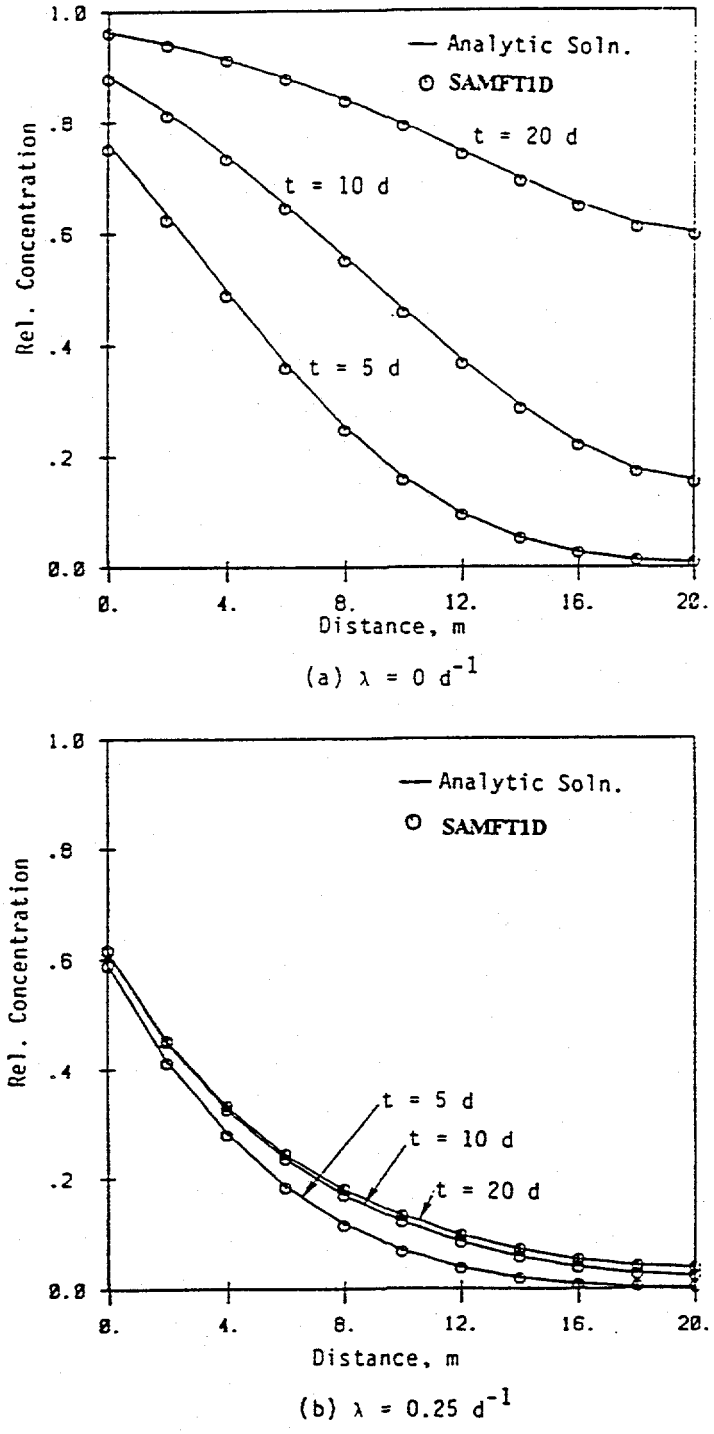


Figure 4.14 Simulated concentration profiles for two cases of the problem of solute transport in a soil column of finite length.

4.4 MULTIPHASE FLOW PROBLEMS

4.4.1 Horizontal Two-Phase Flow without Capillary Effect

The first test problem is the classical one-dimensional Buckley-Leverett problem for which an analytical solution is available (Buckley and Leverett, 1942). In this solution both fluids and porous material are assumed to be incompressible, and capillary effects are ignored. The geometry and boundary conditions of the flow domain are shown in Figure 4.15. The system is initially saturated with water (S_w = 0.2) and NAPL "oil" (S_n = 0.8), water is injected with a constant injection rate at the inlet, x=0 from t=0. The flow cross-sectional area is 10 m^2. On the outlet boundary, x = 305m, the pressures for the two fluids are kept to be at zero reference pressures.

The properties of formation and fluids are summarized in Table 4.5. Data used in this simulation are extracted from the work of Nilkuha and Huyakorn (1980). The relative permeability functions used are as follows:

$$k_{rw} = \left[\frac{S_w - S_{wr}}{1 - S_{wr} - S_{nr}} \right]^2 \qquad (4.5)$$

and

$$k_{rn} = \left[\frac{1 - S_w - S_{nr}}{1 - S_{wr} - S_{nr}} \right]^2 \qquad (4.6)$$

for $S_{wr} < S_w < 1 - S_{nr}$.

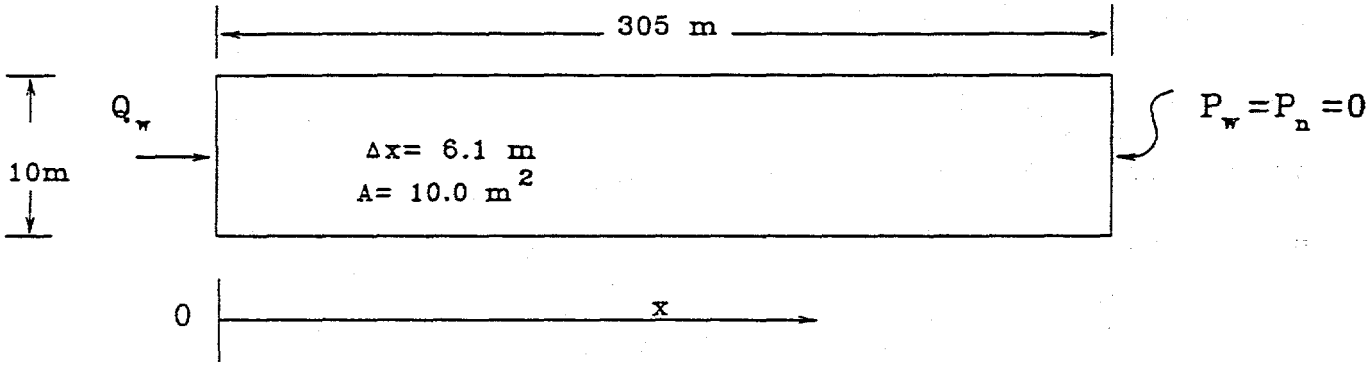


Figure 4.15 Geometry and boundary conditions used in the simulation of the Buckley-Leverett flow problem in a horizontal one-dimensional system.

Table 4.5 Formation and Fluid Properties Used in the Simulation of the Buckley-Leverett Flow Problem for Test 1.

PARAMETER	VALUE
Permeability, k	0.3×10^{-12} m^2
Initial Porosity, ϕ_o	0.20
Cross-Sectional Area, A	10.0 m^2
Residual Water Saturation, S_{wr}	0.20
Irreducible NAPL Saturation, S_{nr}	0.20
Water Viscosity, μ_w	86.4 kg/(m-d)
NAPL Viscosity, μ_n	86.4 kg/(m-d)
Water Injection Rate, Q_w	0.13 m^3/d
Initial Water Density, ρ_w°	1000 kg/m^3
Initial NAPL Density, ρ_n°	1000 kg/m^3
Water Compressibility, C_w	3×10^{-20} (kg/md^2)$^{-1}$
NAPL Compressibility, C_n	3×10^{-20} (kg/md^2)$^{-1}$
Porous Compressibility, C_r	5×10^{-20} (kg/md^2)$^{-1}$

If $S_w \geq 1 - S_{nr}$,

$$\left.\begin{aligned} k_{rw} &= 1 \\ k_{rn} &= 0 \end{aligned}\right\} \tag{4.7}$$

and if $S_w \leq S_{wr}$,

$$\left.\begin{aligned} k_{rw} &= 0 \\ k_{rn} &= 1 \end{aligned}\right\} \tag{4.8}$$

The linear flow domain is discretized using block-centered grids with 50 elements, and a constant mesh spacing ($\Delta x = 6.1$ m) is used. For convenience, the formation is assumed to be homogeneous with constant permeability and initial porosity, as given in Table 4.5. The simulation is performed for 60 time steps. The time step values are generated within the code using the algorithm: $\Delta t_1 = 20$ d, $\Delta t_n = 1.2\ \Delta t_{n-1} \leq 80$ d for $n = 2, 3, \ldots 60$. Relative convergence tolerance criteria are used, and the maximum allowable relative errors for pressure and saturation are 0.01 for this case.

A comparison of the water saturation profiles calculated from SAMFT1D and the Buckley-Leverett analytical solution after 967 d of water injection is shown in Figure 4.16. This indicates that the numerical results from SAMFT1D are in good agreement with the analytical solution considering that very large time steps and grids are used. The analytical solution is evaluated using the computerized graphic method of Welge (1952), programmed by Wu, Pruess and Chen (1990).

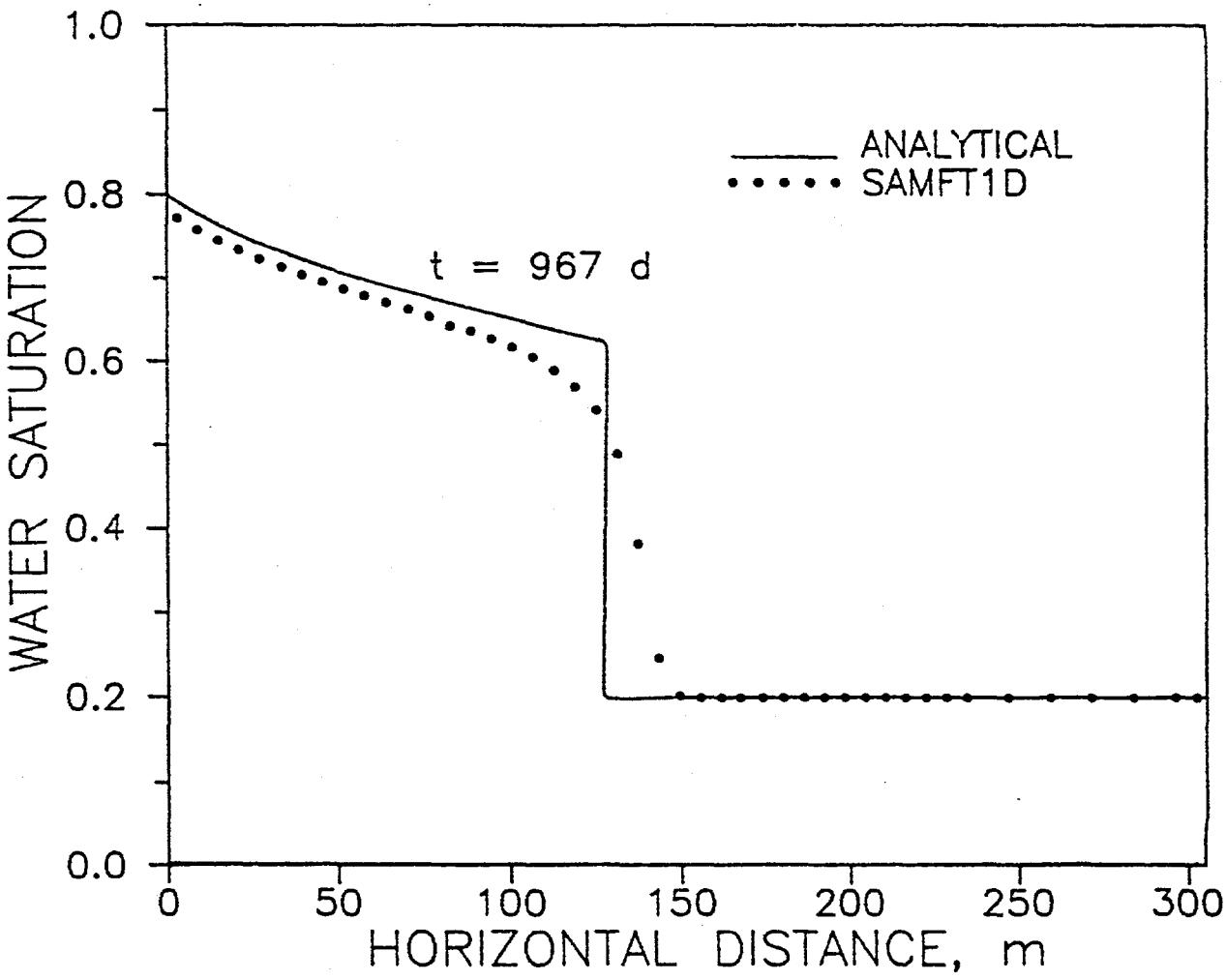


Figure 4.16 Comparison of water saturation profiles calculated from analytical and numerical solutions for horizontal two-phase water and NAPL flow.

4.4.2 Vertical Two-Phase Flow without Capillary Effect

This second test problem concerns two-phase flow through a vertical sand column. If capillary effects are negligible, the Buckley-Leverett type analytical solution is also available in the literature (Wu, Pruess and Chen, 1990) to examine the numerical solutions. Geometry and boundary conditions for this test are described in Figure 4.17. In this case, all of fluid and porous medium properties, flow system dimensions, initial conditions, and constitutive equations for relative permeability are almost identical to those in the previous test problem. Only changes made are: 1) initial NAPL density is $\rho_n^\circ = 864$ kg/m^3, and 2) initial pressures are at hydrostatic condition, i.e., on the bottom boundary, pressures of the two phases are given by the weight of a 305 meter water column.

As shown in Figure 4.17, the flow system is subject to water flux at the top, and constant pressures at the bottom. The same grids and time-steps generation or reduction options as in Test 1 are used for this case. Computed water saturation after 900 days of water injection by SAMFT1D and a comparison with the Buckley-Leverett type analytical solution are shown in Figure 4.18, and good agreement has been obtained between the numerical and analytical solutions for this vertical downward flow case.

The displacement of the two phases near the top of the column shows a vertical straight line of saturation versus depth by the analytical solution. Physically, this means that the only flowing phase is water since water fractional flow is equal to one there, and that NAPL becomes immobile from strong gravity effects. Numerically, this is very difficult because NAPL flux reduces to zero under buoyancy force from water. However, the numerical solution, as shown

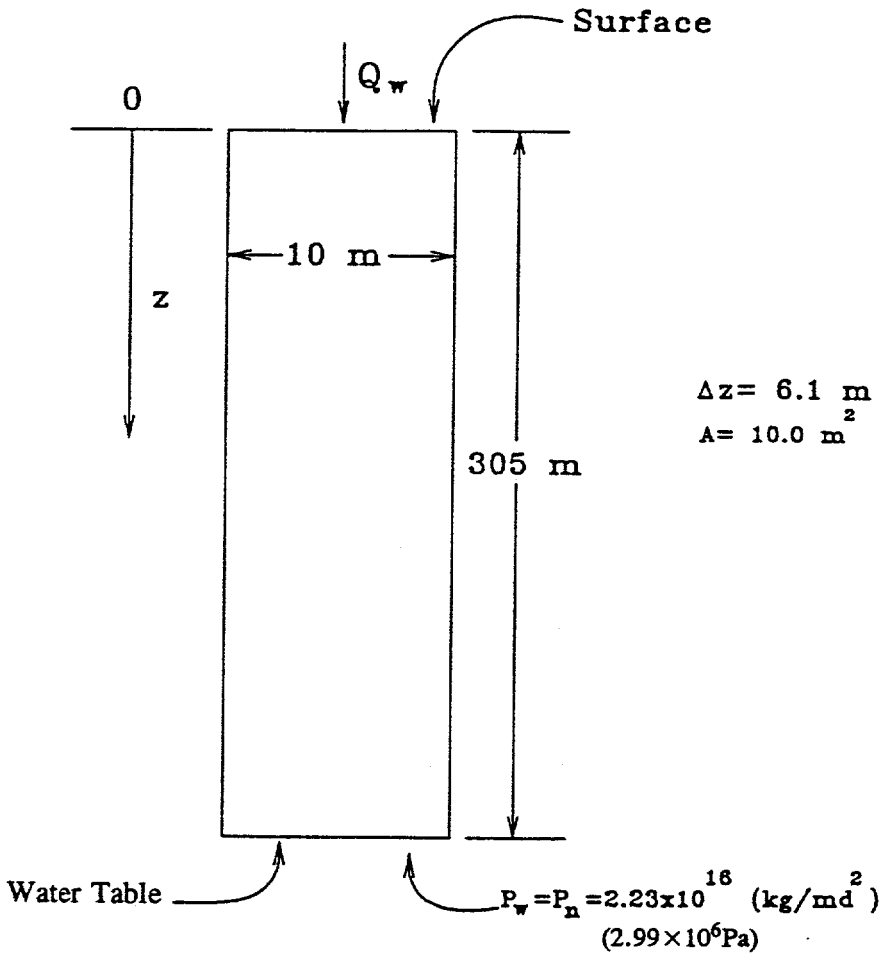


Figure 4.17 Geometry and boundary conditions used in the simulation of the two-phase flow problem in a vertical one-dimensional system.

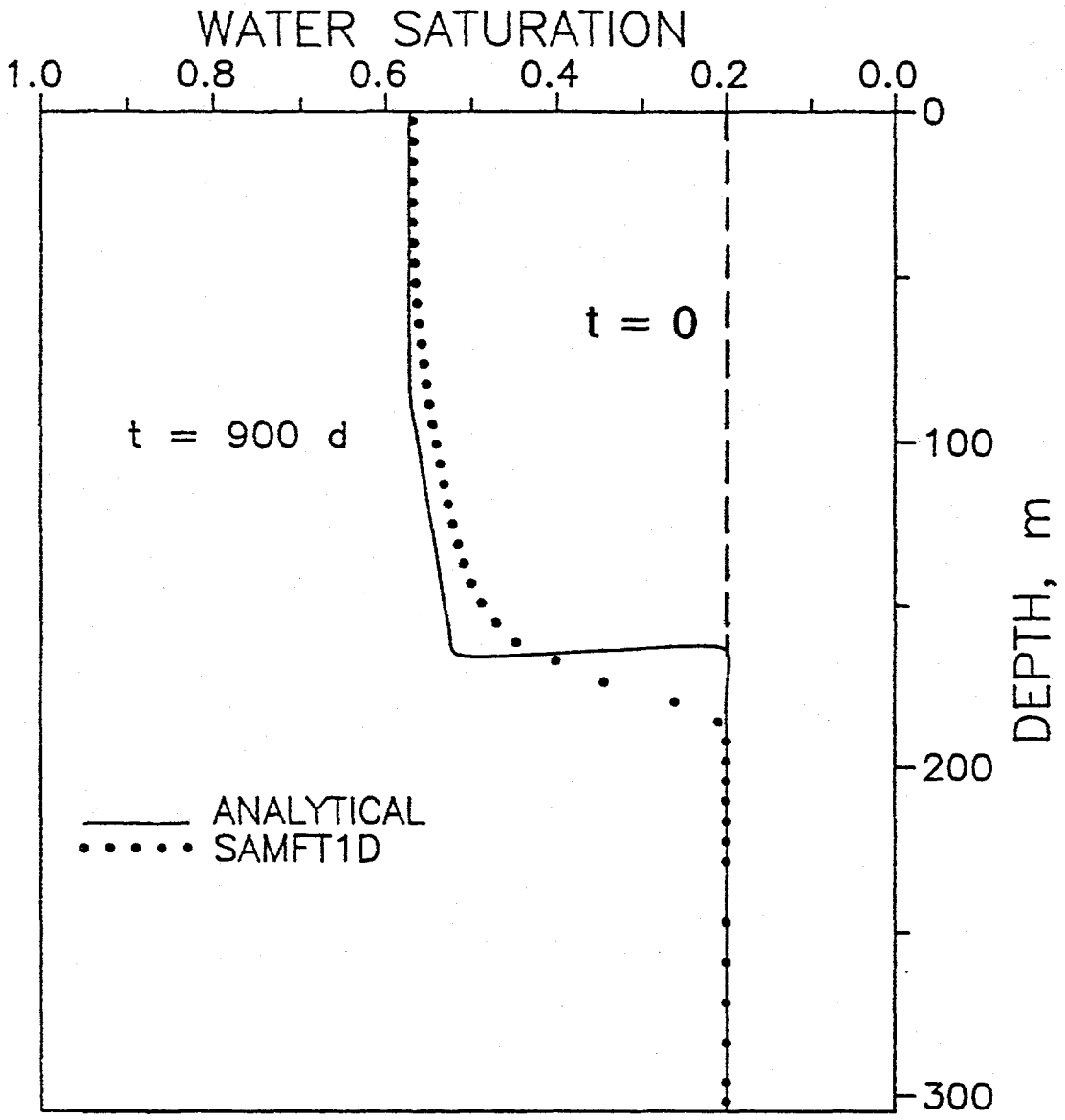


Figure 4.18 Comparison of water saturation profiles calculated from analytical and numerical solution for vertical two-phase water and NAPL flow.

in Figure 4.18, captures this phenomenon very well, and this indicates that the numerical model correctly describes the multiphase immiscible displacement with gravity effects in porous media.

4.4.3 Horizontal Two-Phase Flow with Capillary Effect

The third test problem is to demonstrate that the SAMFT1D code yields the correct solution when including effects of capillary pressure. This test uses an analytical solution with capillary effects recently developed by McWhorter and Sunada (1990), and the data of the analytical solution are from Kueper (1989).

The physical problem for this code verification example involves a one-dimensional, horizontal column of incompressible porous media, initially fully saturated by an incompressible wetting fluid, water. Another non-wetting incompressible fluid, NAPL, is continuously injected at the inlet end of the column for $t > 0$ at a rate such that a constant saturation S_w^o is maintained at this boundary,

$$S_w(o,\ t) = S_w^o, \qquad t > 0 \tag{4.9}$$

to achieve a constant saturation, the wetting phase pressure drop across the column must delay as a function of time,

$$P_w(o, t) - P_w(L, t) = \frac{C_1}{\sqrt{t}} - C_2, \qquad t \le t^o \tag{4.10}$$

where C_1 and C_2 are constants, and t^o is the time when the injected fluid first reaches the outlet end of the column ($x = L$). The analytical solution also requires at the inlet end, wetting phase injection flux is zero (Kueper, 1989).

$$Q_w(0, t) = 0, \qquad t > 0 \tag{4.11}$$

This is not a reasonable condition physically. However, we can complement it in the numerical code without much difficulty.

Capillary pressure and relative permeability curves are chosen to be in functional forms (Honarpour, et. al., 1986). For capillary pressure, a Brooks-Corey curve is used as

$$P_c = \frac{P_d}{S_e^{1/\lambda}} \tag{4.12}$$

where P_d is the displacement pressure corresponding to the capillary pressure which first gives rise to non-wetting phase permeability, λ is a pore size distribution index, S_e is an effective saturation, defined as:

$$S_e = \frac{S_w - S_{wr}}{1 - S_{wr}} \tag{4.13}$$

The relative permeability to wetting phase is specified as:

$$k_{rw} = S_e^{\frac{2+3\lambda}{\lambda}} \tag{4.14}$$

and the relative permeability to the non-wetting phase as:

$$k_{rn} = (1 - S_e)^2 \left(1 - S_e^{\left(\frac{2+\lambda}{\lambda}\right)}\right) \tag{4.15}$$

The fluid and porous medium properties are given in Table 4.6, and the flow geometry and boundary conditions of a 10 meter long column are shown in Figure 4.19. In order to satisfy the conditions for the analytical solution, both pressure and flux boundary conditions are

Table 4.6 Formation and Fluid Properties Used in the Simulation of Horizontal Two-Phase Flow with Capillary Effects for Test 3.

PARAMETER	VALUE
Permeability, k	5×10^{-11} m^2
Initial Porosity, ϕ_o	0.35
Cross-Sectional Area, A	1.0 m^2
Column Length, L	10.0 m
Residual Water Saturation, S_{wr}	0.05
Inlet Water Saturation, S_w°	0.525
Pore Size Index, λ	2.0
Outlet Water Pressure, $P_w(L,t)$	0.0
Water Viscosity, μ_w	1×10^{-3} Pa.s
NAPL Viscosity, μ_n	0.5×10^{-3} Pa.s
Initial Water Density, ρ_w°	1000 kg/m^3
Initial NAPL Density, ρ_n°	1000 kg/m^3
Water Compressibility, C_w	5×10^{-10} Pa^{-1}
NAPL Compressibility, C_n	5×10^{-10} Pa^{-1}
Porous Compressibility, C_r	5×10^{-10} Pa^{-1}
Constant, C_1	1.339×10^5 kg/m.s$^{3/2}$
Constant, C_2	-89.7 Pa

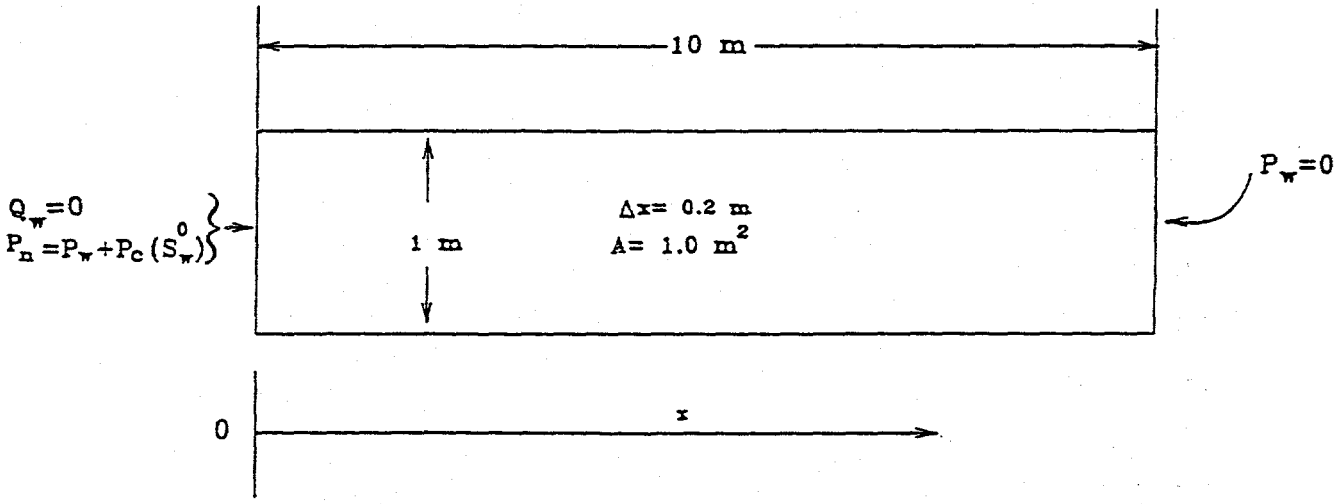


Figure 4.19 Geometry and boundary conditions used in the simulation of the two-phase flow with capillary effects in a horizontal one-dimensional system.

proposed on the inlet, as shown in Figure 4.19, which are not generally required for application problems since pressure and flux cannot be controlled simultaneously at the same boundary. The NAPL injection pressure at the inlet end is calculated by

$$\begin{aligned} P_n(0,t) &= P_w(0,t) + P_c(S_w^o) \\ &= 2828.43 + P_w(0,t) \end{aligned} \tag{4.16}$$

Since the pressure at the inlet end changes with time, and it tends to be infinite as t approaches zero, from Eq. 4.10, the pressure boundary condition at x=0 is treated as a discretized function of time. The values of time and NAPL pressures are given in Table 4.7, which are used in the simulation to approximate the pressure boundary condition by Eq. (4.19).

The flow domain is discretized using 50 block-centered grids of the same size ($\Delta x = 0.2$ m). The simulation is performed for 100 time steps. The first time step, $\Delta t_1 = 1000$ s, and maximum time step used is 1×10^6 s. The relative convergence tolerance for pressure and saturation is 0.01. Figure 4.20 presents the comparison of effective saturation from the analytical solution and SAMFT1D at three different injection times. The agreement between analytical and numerical solution is very good. Only at the leading edge of the displacement front does the numerical solution deviate somewhat from the analytical solution, which is typical of "smearing" effects from numerical dispersion.

4.4.4 Horizontal Two-Phase Imbibition with Capillary Effect

This test problem is a horizontal flow problem with water imbibition into an unsaturated porous medium. The example is taken from the study on the Topapah Spring Welded Tuff unsaturated zone, below Yucca Mountain in Nevada, a possible site for an underground

Table 4.7 Prescribed Values of Time and NAPL Pressures at the Inlet End.

t (s)	P_n (Pa)	t (s)	P_n (Pa)
0	10,000.0	6,000	4,467.4
500	8,727.2	7,000	4,339.2
1,000	6,973.2	8,000	4,235.8
1,500	6,196.2	9,000	4,150.2
2,000	5,732.9	10,000	4,077.8
2,500	5,417.8	20,000	3,685.6
3,000	5,183.5	50,000	3,337.6
3,500	5,002.2	100,000	3,162.2
4,000	4,855.9	500,000	2,928.1
4,500	4,734.8	1,000,000	2,872.1
5,000	4,632.4	10,000,000	2,781.1

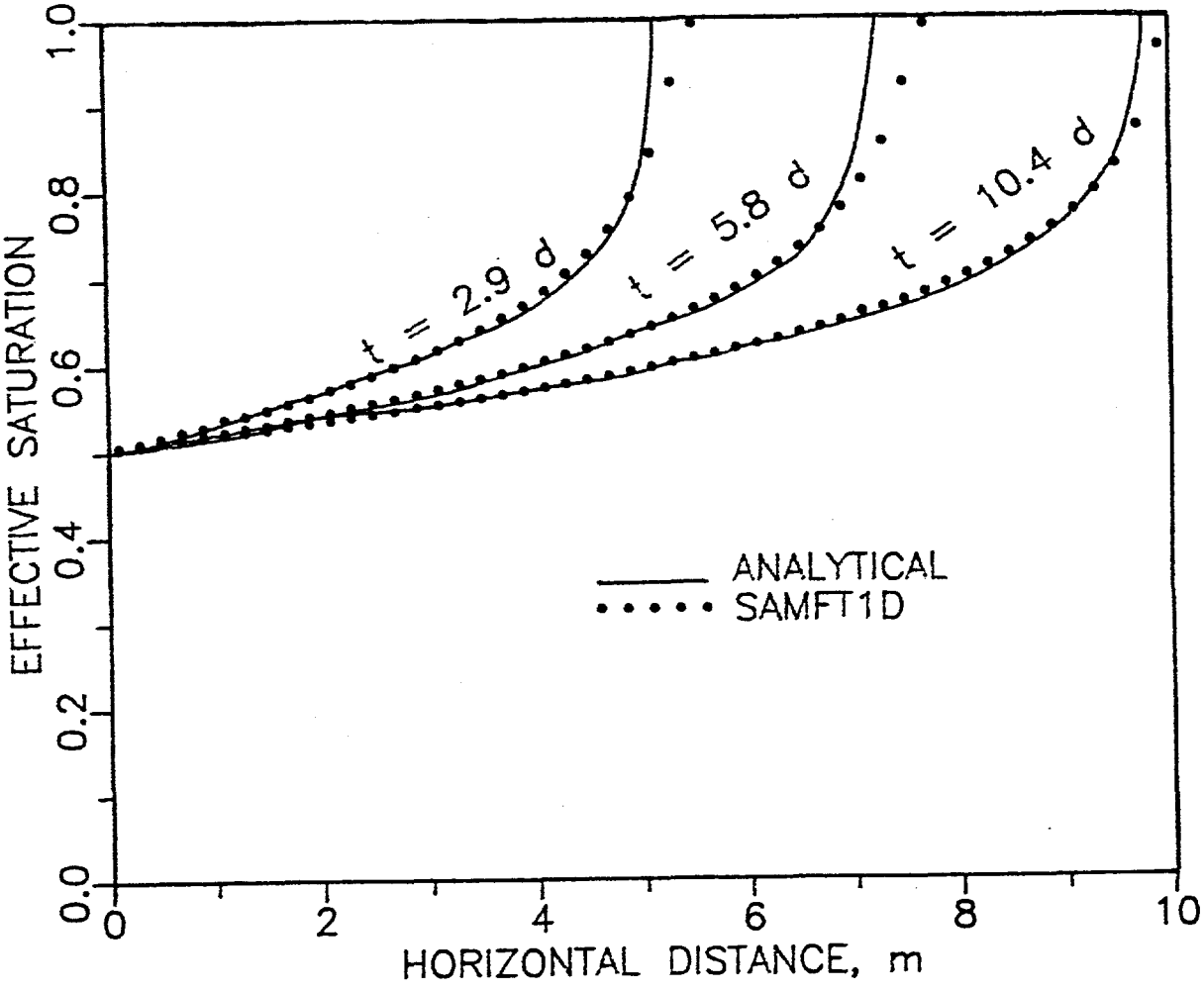


Figure 4.20 Comparison of effective saturations calculated from analytical and numerical solutions for horizontal two-phase flow with capillary effects.

nuclear waste repository. This imbibition problem has been used as a test case for a similarity solution (Zimmerman and Bodvarsson, 1989), an exact integral solution (Chen, Zimmerman and Bodvarsson, 1990) of two-phase flow, and also been solved using the TOUGH code (Pruess, 1987).

The relative permeability to water phase and capillary pressure functions are taken as:

$$k_{rw} = \left[1 - (1 - s_e^{1.49})^{0.671}\right]^2 \sqrt{S_e} \tag{4.17}$$

and

$$P_c = 0.872 \times 10^5 \left[S_e^{-1.49} - 1\right]^{0.329} \quad Pa \tag{4.18}$$

where S_e is defined as:

$$S_e = \frac{S_w - S_{wr}}{S_w^* - S_{wr}} \tag{4.19}$$

and S_w^* is maximum obtainable water saturation. These equations are of the forms proposed by van Genuchten (1980), and were used by Chen et. al. (1990). Since we use two-phase flow equations to solve the problem, a relative permeability function for the air phase is needed, which is,

$$k_{ra} = 1 - k_{rw} \tag{4.20}$$

Geometry and boundary conditions of the imbibition system are shown in Figure 4.21. The one-meter flow domain is uniformly saturated with water and air initially, and is discretized using a 25-block grid with uniform nodal spacings of 0.04 m. The initial water pressure is -1 $\times$ 10^5 Pa and the air pressure is zero under equilibrium conditions. On the inlet boundary

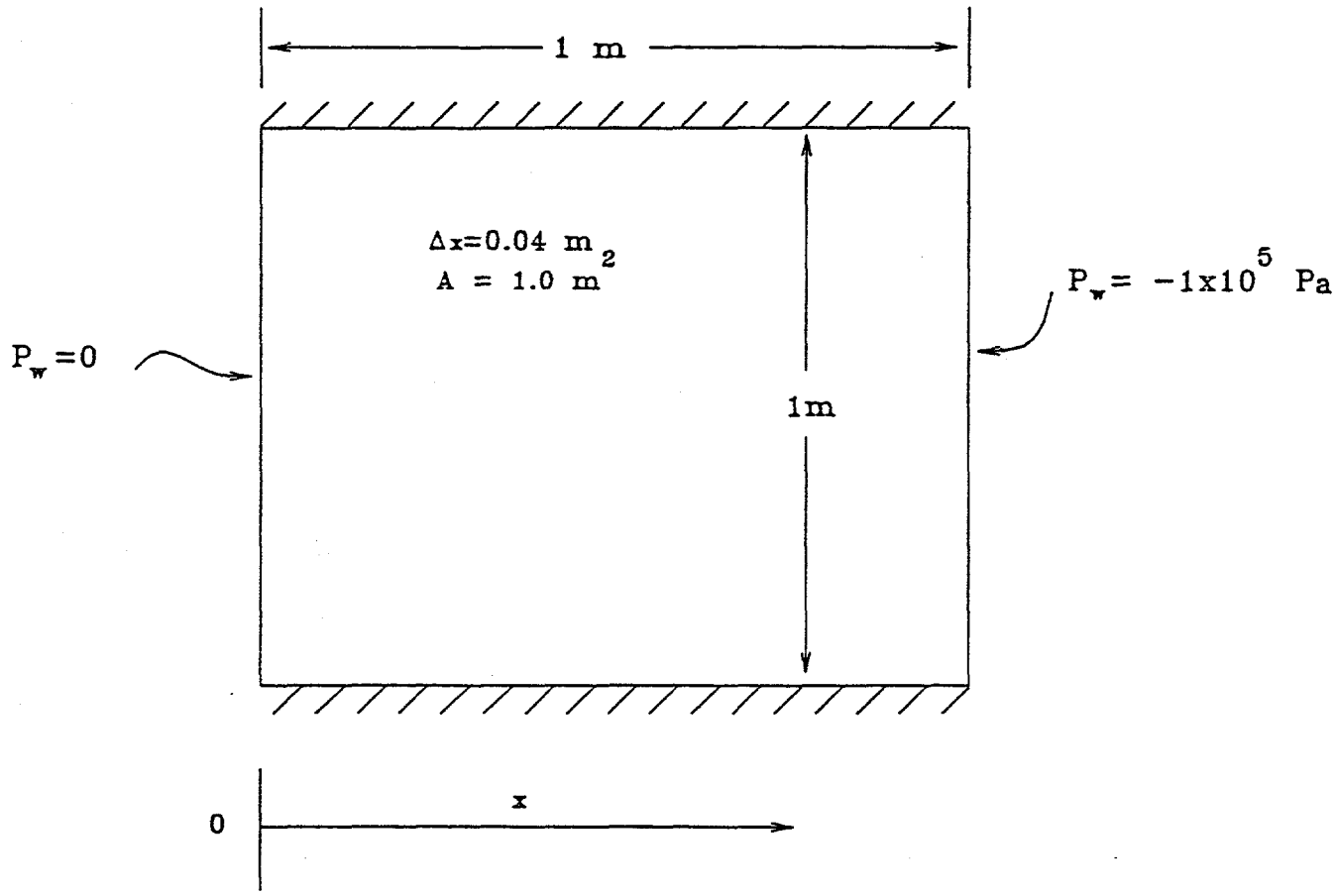


Figure 4.21 Geometry and boundary conditions in the simulation of water imbibition in a horizontal one-dimensional system.

(x=0), the water phase pressure is prescribed as zero. On the outlet end, the water pressure is kept constant and equal to the initial value of -1×10^5 Pa.

The parameter values for the fluids and porous media are summarized in Table 4.8. In this case, water imbibition is due to capillary pressure, and very strong capillary effects are expected. The relative convergence tolerances for pressure and saturation are set as 0.005 and the first time step is chosen to be 1000 s. The simulation result and the analytical solution (Chen, et. al., 1990) are compared in Figure 4.22 for water saturation profiles at an elapsed time of 1×10^7 s (116 d). The agreement between the numerical calculation by SAMFT1D and the analytical solution is very good.

4.4.5 Vertical Two-Phase Flow in a Three-Phase System

This simple problem is designed to test the capability of the code SAMFT1D to handle immiscible fluid flow within and below the unsaturated zone including effects of gravity and capillary pressure. In this case, the air phase is treated as a passive phase, and the pressure in the air phase is assumed to be atmospheric. The test example is taken from the work of Faust (1985), and here we simplify it to a one-dimensional problem. The flow domain and conditions are shown in Figure 4.23. This 5-meter soil column contains both saturated and unsaturated zones with initial water table 1.5 meter below the surface. The surface boundary is subject to simultaneous injection of water and NAPL, and the bottom boundary is subject to a constant pressure. The physical parameters for the simulation are given in Table 4.9.

The one-dimensional flow domain was discretized into 20 elements using block-centered grids and a constant mesh spacing ($\Delta z = 0.25$ m). The initial condition generated by the code

Table 4.8 Formation and Fluid Properties Used in the Simulation of Horizontal Two-Phase Imbibition with Capillary Effect.

PARAMETER	VALUE
Permeability, k	3.9×10^{-18} m^2
Initial Porosity, ϕ_o	0.14
Cross-Sectional Area, A	1.0 m^2
Column Length, L	1.0 m
Residual Water Saturation, S_{wr}	0.318
Maximum Water Saturation, S_w^*	0.984
Initial Water Saturation, S_{wi}	0.676
Water Viscosity, μ_w	1×10^{-3} Pa.s
Air Viscosity, μ_a	1.98×10^{-5} Pa.s
Initial Water Density, ρ_w°	1000 kg/m^3
Initial Air Density, ρ_a°	1.18 kg/m^3
Water Compressibility, C_w	2×10^{-10} Pa^{-1}

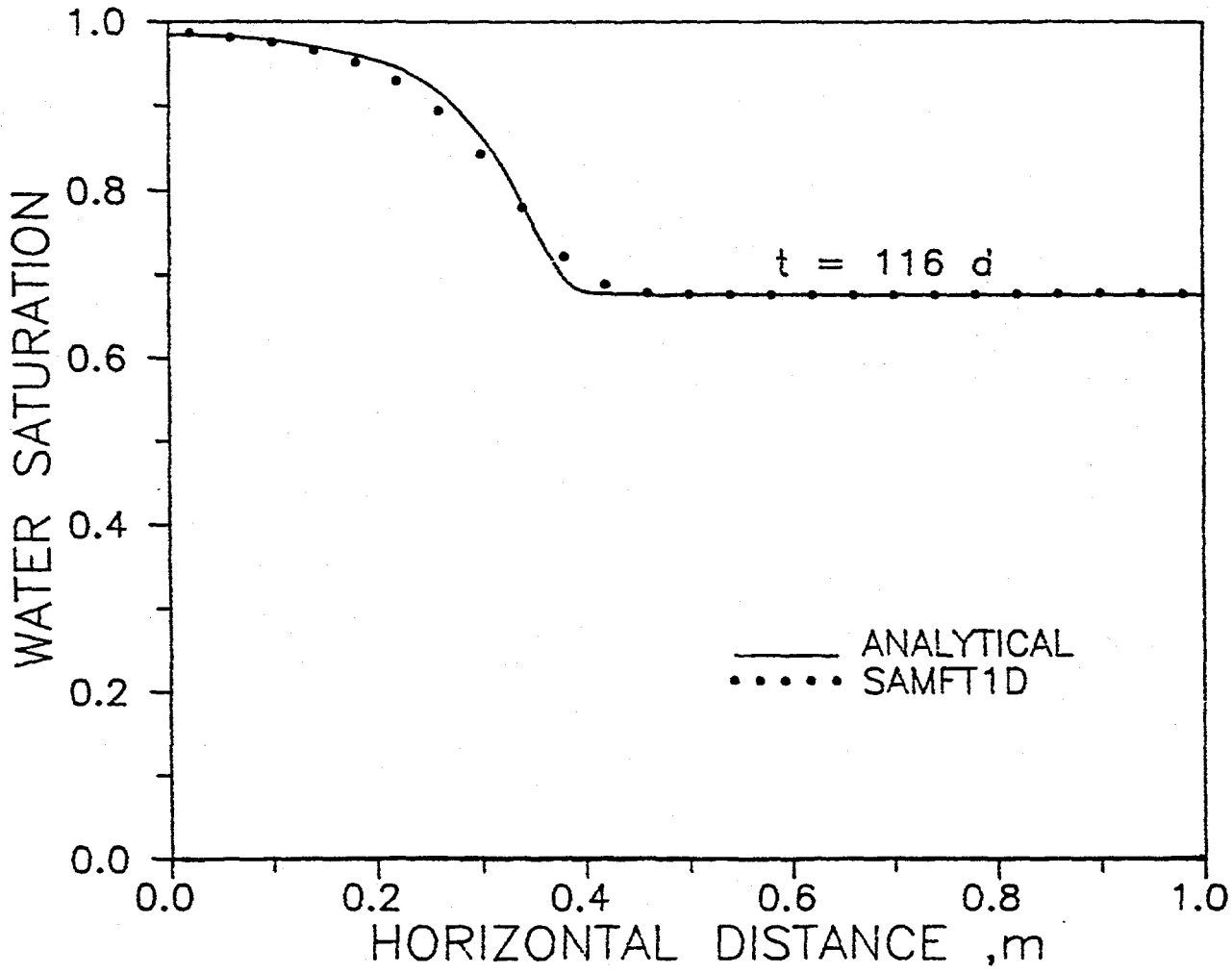


Figure 4.22 Comparison of water saturations calculated from analytical and numerical solutions for horizontal two-phase imbibition with capillary effects.

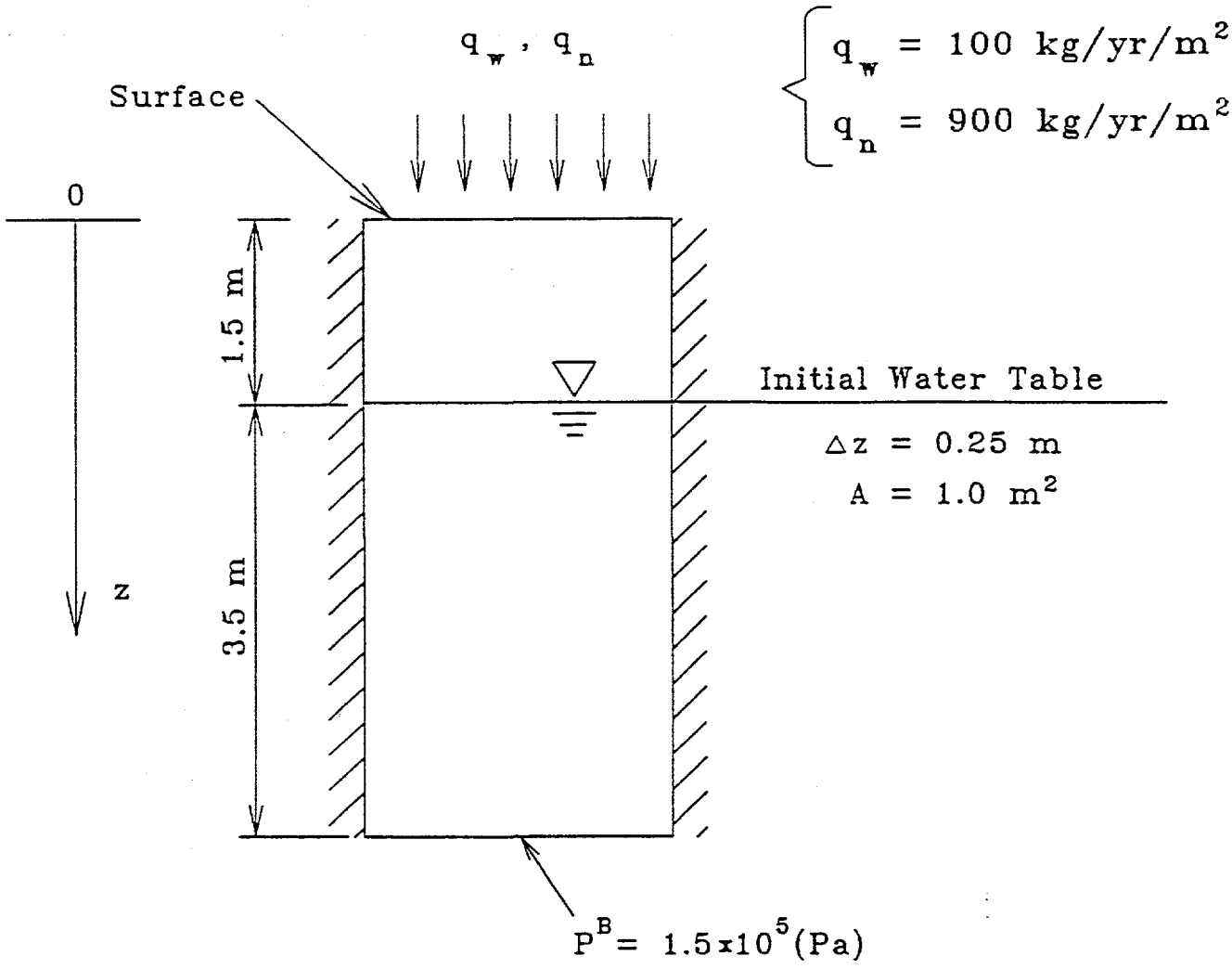


Figure 4.23 Geometry and boundary conditions in the simulation vertical two-phase flow in a three-phase system.

Table 4.9 Soil and Fluid Properties Used in the Simulation of Two-Phase Flow in a Three-Phase System.

PARAMETER	VALUE
Permeability, k	1×10^{-12} m^2
Initial Porosity, ϕ_o	0.3
Cross-Sectional Area, A	1.0 m^2
Column Length, L	5.0 m
Depth to Water Table, H	1.5 m
Atmospheric Pressure, P_{atm}	10^5 Pa
Initial Water Density, ρ_w°	1,000 kg/m^3
Initial NAPL Density, ρ_n°	950 kg/m^3
Water Viscosity, μ_w	1×10^{-3} Pa.s
NAPL Viscosity, μ_n	1×10^{-3} Pa.s
Water Compressibility, C_w	4.3×10^{-9} Pa^{-1}
NAPL Compressibility, C_n	3.0×10^{-9} Pa^{-1}
Porous Compressibility, C_r	10^{-10} Pa^{-1}
Water Injection Rate, Q_w	100 kg/yr
NAPL Injection Rate, Q_n	900 kg/yr
Bottom Pressure, P^B	1.5×10^5 Pa

is given in Table 4.10, and relative permeability and capillary pressure data used by Faust (1986) and (Forsyth, 1990) in the two-dimensional simulation of the same problem are shown in Table 4.11. The simulation was performed for 60 time steps. The time steps were generated by the code using the scheme outlined in Section 3.3.4.b. The initial and maximum time steps used are $\Delta t_1 = 0.115$ d, and $\Delta t_{max} = 50$ d. The maximum time step was reached after 35 time steps. The final time value of the run after 60 time step simulations is 1,700 days for this problem.

In order to verify the computational modules of SAMFT1D for modeling two-phase fluid flow under three-phase conditions, the simulation results of SAMFT1D are compared with the results from the three-dimensional numerical model (NAPL3D) of Forsyth (1990). The comparison of NAPL and water saturations from SAMFT1D and NAPL3D at five time values from 10 to 500 days are shown in Figures 4.24 and 4.25, respectively. The agreement of the results from the present model and NAPL3D is excellent for the entire simulation time period.

4.4.6 Vertical Three-Phase Flow

This is the problem designed to test the SAMFT1D code under the condition that all three fluid phases (water, NAPL and air) are active. The flow domain and problem description are the same as problem 4.4.5. Also, the same parameters, initial conditions (Table 4.10), and relative permeability and capillary pressure data (Table 4.11) are used in this case. However, one additional surface boundary condition is needed for the air flow equation, and a zero flux condition was used in this case, i.e., no air is allowed to cross the surface boundary. The

Table 4.10 Initial Conditions Used in the Simulation of Two-Phase Flow in a Three-Phase System.

Node	P_n (Pa)	S_w	S_n
1	0.9850E+05	0.8500E+00	0.0000
2	0.9877E+05	0.8773E+00	0.0000
3	0.9905E+05	0.9045E+00	0.0000
4	0.9932E+05	0.9318E+00	0.0000
5	0.9959E+05	0.9591E+00	0.0000
6	0.9986E+05	0.9864E+00	0.0000
7	0.1012E+06	0.1000E+01	0.0000
8	0.1037E+06	0.1000E+01	0.0000
9	0.1061E+06	0.1000E+01	0.0000
10	0.1086E+06	0.1000E+01	0.0000
11	0.1110E+06	0.1000E+01	0.0000
12	0.1135E+06	0.1000E+01	0.0000
13	0.1159E+06	0.1000E+01	0.0000
14	0.1184E+06	0.1000E+01	0.0000
15	0.1208E+06	0.1000E+01	0.0000
16	0.1233E+06	0.1000E+01	0.0000
17	0.1257E+06	0.1000E+01	0.0000
18	0.1282E+06	0.1000E+01	0.0000
19	0.1306E+06	0.1000E+01	0.0000
20	0.1331E+06	0.1000E+01	0.0000

Table 4.11 Relative Permeability and Capillary Pressure Data Used in the Simulation of Two-Phase Flow in a Three-Phase System.

Water and NAPL Two-Phase System

S_w	k_{rw}	k_{rn}^{wn}	P_{cnw}(Pa)
0.2	0.00	0.68	0.90×10^4
0.3	0.04	0.55	0.54×10^4
0.4	0.10	0.43	0.39×10^4
0.5	0.18	0.31	0.33×10^4
0.6	0.30	0.20	0.30×10^4
0.7	0.44	0.12	0.27×10^4
0.8	0.60	0.05	0.24×10^4
0.9	0.80	0.00	0.15×10^4
1.0	1.00	0.00	0.00

Liquid and Air System

S_a	k_{ra}	k_{rn}^{n}	P_{can}(Pa)	P_{caw}(Pa)
0.00	0.00	0.680	0.00×10^3	0.00×10^4
0.10	0.01	0.490	0.90×10^3	0.10×10^4
0.20	0.04	0.340	0.12×10^4	0.20×10^4
0.30	0.09	0.210	0.15×10^4	0.30×10^4
0.40	0.16	0.116	0.18×10^4	0.33×10^4
0.50	0.25	0.045	0.21×10^4	0.36×10^4
0.60	0.36	0.009	0.24×10^4	0.39×10^4
0.68	0.46	0.000	0.30×10^4	0.45×10^4
0.80	0.64	0.000	0.90×10^4	0.66×10^4

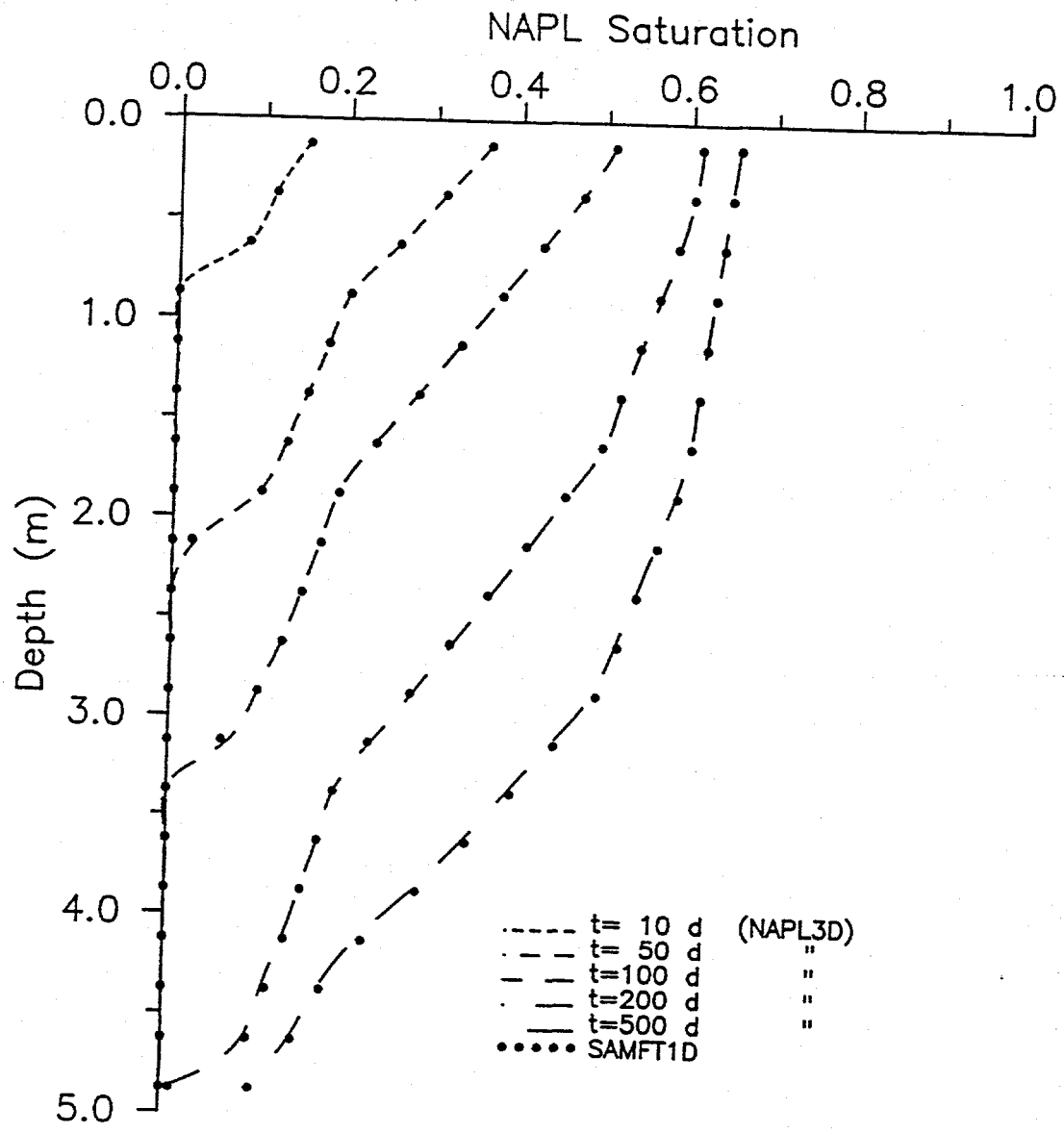


Figure 4.24 Comparison of NAPL saturations calculated from SAMFT1D and NAPL3D (Forsyth, 1990) for two-phase flow under three-phase condition.

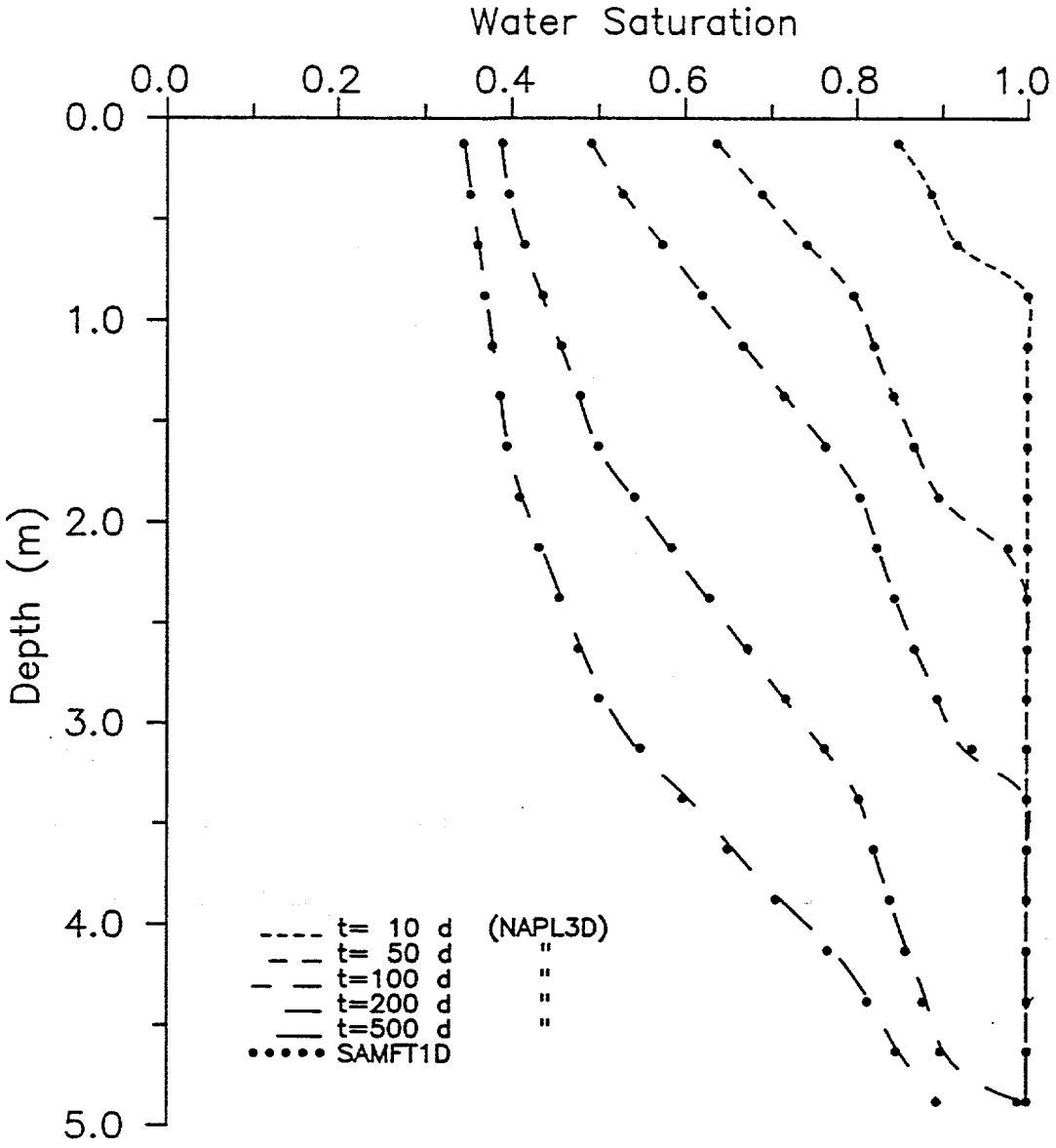


Figure 4.25 Comparison of water saturations calculated from SAMFT1D and NAPL3D (Forsyth, 1990) for two-phase flow under three-phase condition.

automatic time stepping algorithm was also used in this simulation to update time steps. The same initial and maximum time steps as problem 4.4.5 were used, $\Delta t_i = 0.115$ d, and $\Delta t_{max} = 50$ d. In this case, the time step increased to the maximum value of 50 days after only 25 time step runs.

The simulation results for this three-phase flow problem from SAMFT1D were checked against a three-dimensional compositional model by Forsyth and Shao (1991). The comparison of NAPL and water saturations from the two codes is given in Figures 4.26 and 4.27, respectively. The agreement of the simulations is good, as shown in Figures 4.26 and 4.27. However, there is some difference between the saturation results in the nodes near the top surface. The reason is that the data used in the compositional model is not exactly equivalent to those used by SAMFT1D. The compositional model treats the water as a component which exists in both the water and air phases. In this case, there is 10% water in the air phase. After a few grid blocks from the surface, the results obtained from the two models are in better agreement as can be seen in Figures 4.26 and 4.27. Another interesting observation is that all the air is trapped in the top two elements by buoyancy force, since the air cannot flow out from the top boundary.

4.4.7 Vertical Three-Phase Flow with Pulse Release of NAPL on the Surface

The purpose of this problem is to test the performance of SAMFT1D in modeling a more complex unsaturated zone contamination case involving a pulse release of NAPL from the ground surface and including effects of gravity and capillary pressure forces. This is a typical

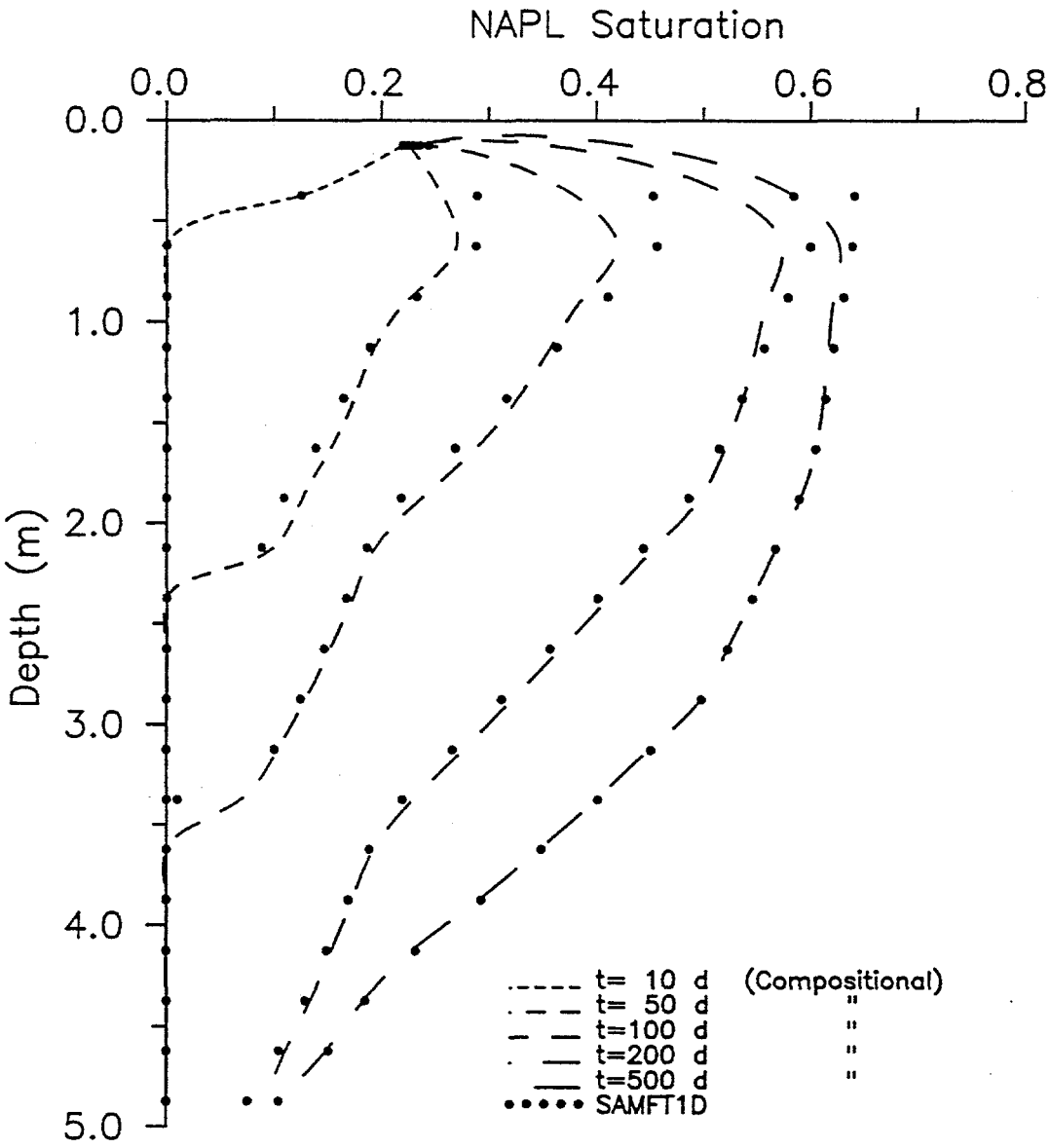


Figure 4.26 Comparison of NAPL saturations calculated from SAMFT1D and compositional model (Forsyth and Shao, 1991).

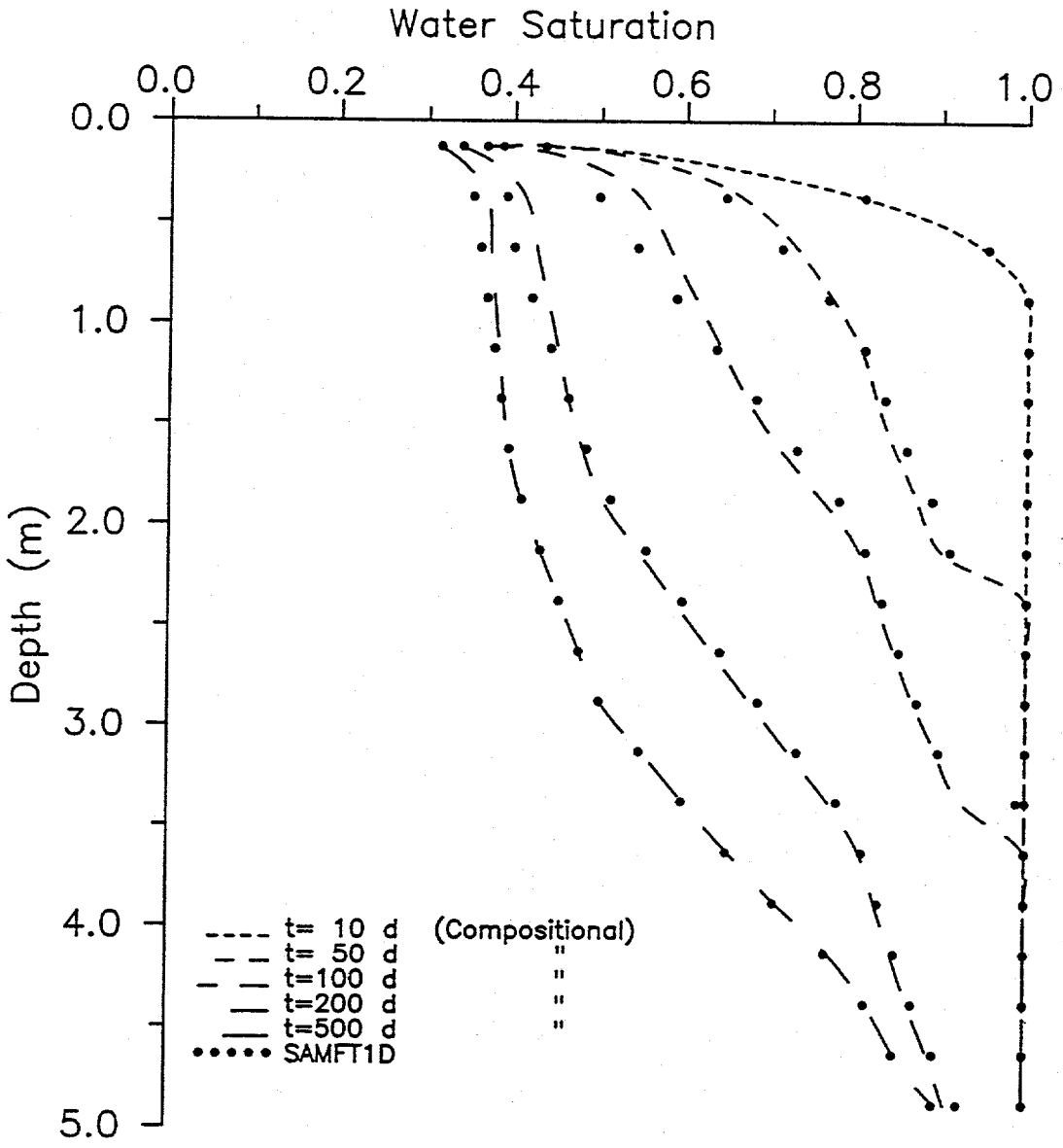


Figure 4.27 Comparison of water saturations calculated from SAMFT1D and compositional model (Forsyth and Shao, 1991).

situation when an accidental spillage of NAPL on the ground provides a discontinuous contaminant source. The flow domain depicted in Figure 4.28, is a 10-meter vertical soil column above water table. The surface boundary is subjected to water and NAPL injection at t = 0. After 75 days, the NAPL injection stopped, the water injection continued, and the air pressure kept atmospheric all the time. The same physical properties for soil, fluids, relative permeability and capillary pressure data as in Problem 4.4.5 were used. Also, a 20-element grid was employed with a constant grid space (Δz = 0.5 m) to discretize the flow system.

The initial condition was generated by the code using zero fluxes for water and NAPL and $P_a = P_{atm}$ on the top boundary, and water-table conditions on the bottom boundary, respectively, as summarized in Table 4.12. The automatic time stepping scheme was used with the first time step, Δt_1 = 0.115 d, and the maximum time step, Δt_{max} = 100 d. After 100 computational time steps, the simulation time reached 6400 days. The computed values of NAPL saturation for different time values are presented in Figure 4.29. It is interesting to note that the NAPL mass continues to move downward after termination of NAPL injection on the surface at 75 days, as shown in Figure 4.29. The NAPL becomes completely immobile after 500 days, with the front located at a depth of 4 meters. This phenomenon corresponds physically to the equilibrium of gravity and capillary pressure in the non-aqueous phase, which is correctly described by the model.

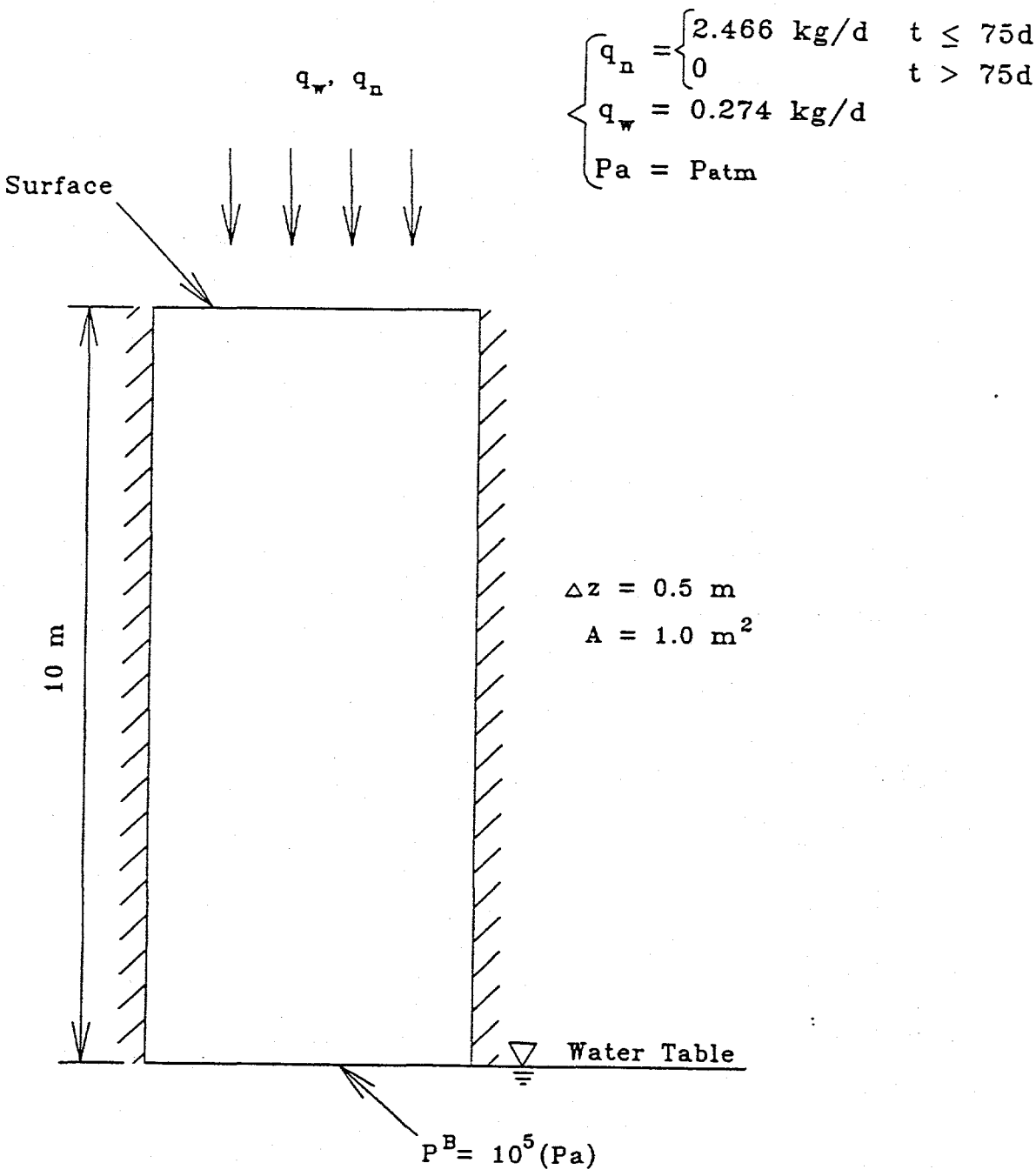


Figure 4.28 Geometry and boundary conditions used in the simulation of three-phase flow with pulse release of NAPL on the surface.

Table 4.12 Initial Condition Used in the Simulation of Three-Phase Flow with Pulse Release of NAPL on the Surface.

Node	P_n (Pa)	S_w	S_n
1	0.9340E+05	0.2000E+00	0.0000
2	0.9340E+05	0.2000E+00	0.0000
3	0.9340E+05	0.2000E+00	0.0000
4	0.9340E+05	0.2000E+00	0.0000
5	0.9340E+05	0.2000E+00	0.0000
6	0.9341E+05	0.2000E+00	0.0000
7	0.9341E+05	0.2000E+00	0.0000
8	0.9341E+05	0.2000E+00	0.0000
9	0.9341E+05	0.2000E+00	0.0000
10	0.9341E+05	0.2000E+00	0.0000
11	0.9341E+05	0.2000E+00	0.0000
12	0.9341E+05	0.2000E+00	0.0000
13	0.9341E+05	0.2000E+00	0.0000
14	0.9341E+05	0.2000E+00	0.0000
15	0.9342E+05	0.2000E+00	0.0000
16	0.9342E+05	0.2000E+00	0.0000
17	0.9342E+05	0.2000E+00	0.0000
18	0.9342E+05	0.2000E+00	0.0000
19	0.9342E+05	0.2000E+00	0.0000
20	0.9755E+05	0.7528E+00	0.0000

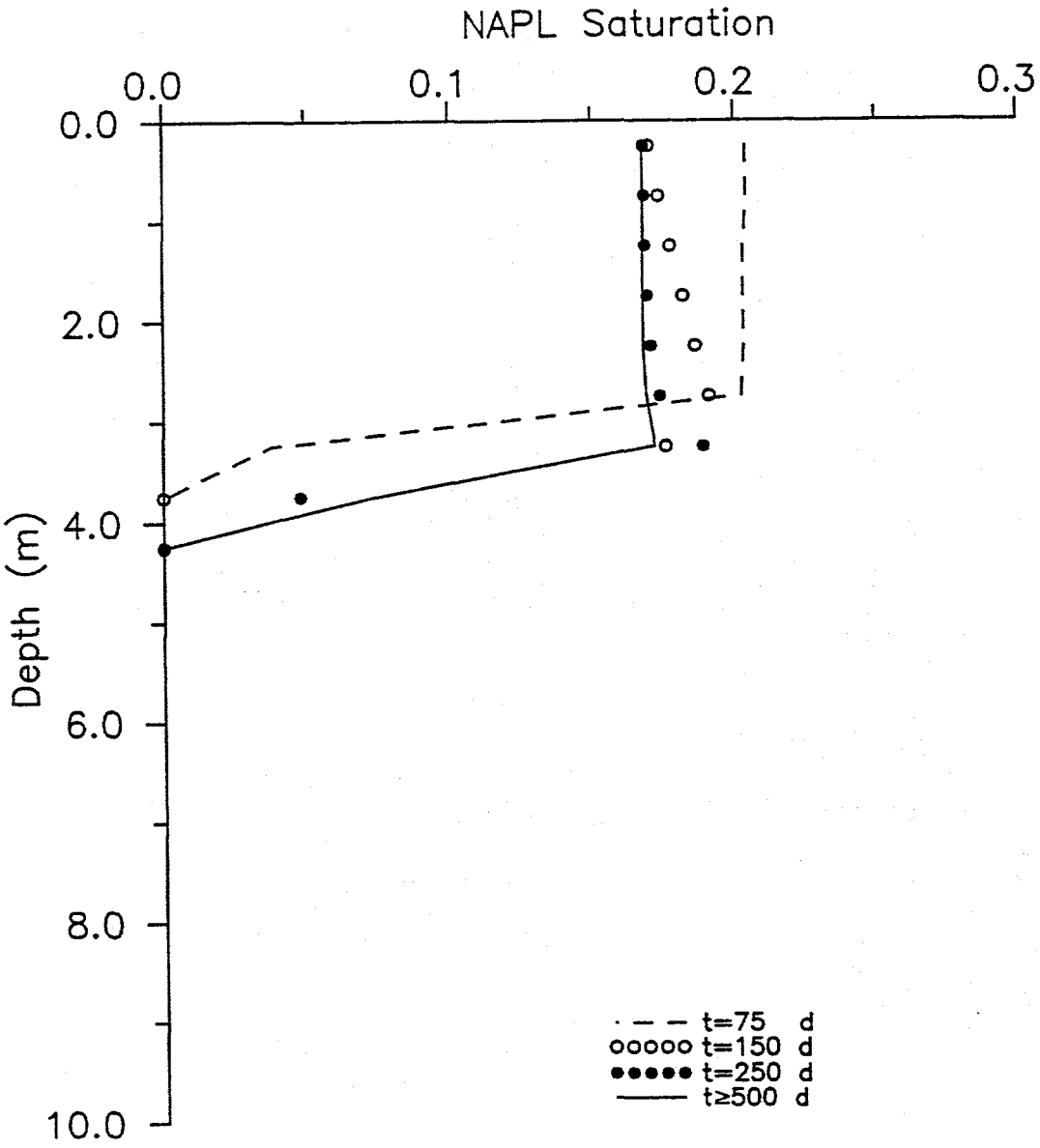


Figure 4.29 Profile of NAPL saturations with the surface boundary subject to pulse release of NAPL.

4.5 MULTIPHASE SOLUTE TRANSPORT EXAMPLES

4.5.1 Two-Phase Examples: Water and Air

In this section, the solute transport computational modules of the SAMFT1D code are verified using selected multiphase transport problems for which analytical solutions can be obtained. It is assumed that there is no NAPL in the system and that the air is stagnant. Furthermore, if the solute is regarded as non-volatile, the problem reduces to that involving single-phase solute transport in one-dimensional uniform groundwater flow for which there exist many known analytical solutions. The purpose of this exercise is then to validate the multiphase solution algorithm against known solutions.

Two example problems are selected. The primary difference between the two is in the boundary conditions: the first one has the specified solute concentration and the second has the specified mass flux at the inflow boundary.

4.5.1.1 Solute Transport in a Semi-infinite Soil Column

This problem concerns one-dimensional transport of a conservative solute species in an unsaturated soil column of 4 m long. The water saturation value in the column is fixed at 0.625. All partition coefficients are assumed to be zero to make the example effectively single phase. The schematic description of the example is given in Figure 4.30. The initial solute concentration in the soil column is assumed to be zero and the solute is introduced into the column from the inlet section at a prescribed solute concentration. The complete listing of the values of physical parameters and discretization data used in the numerical simulation is given in Table 4.13.

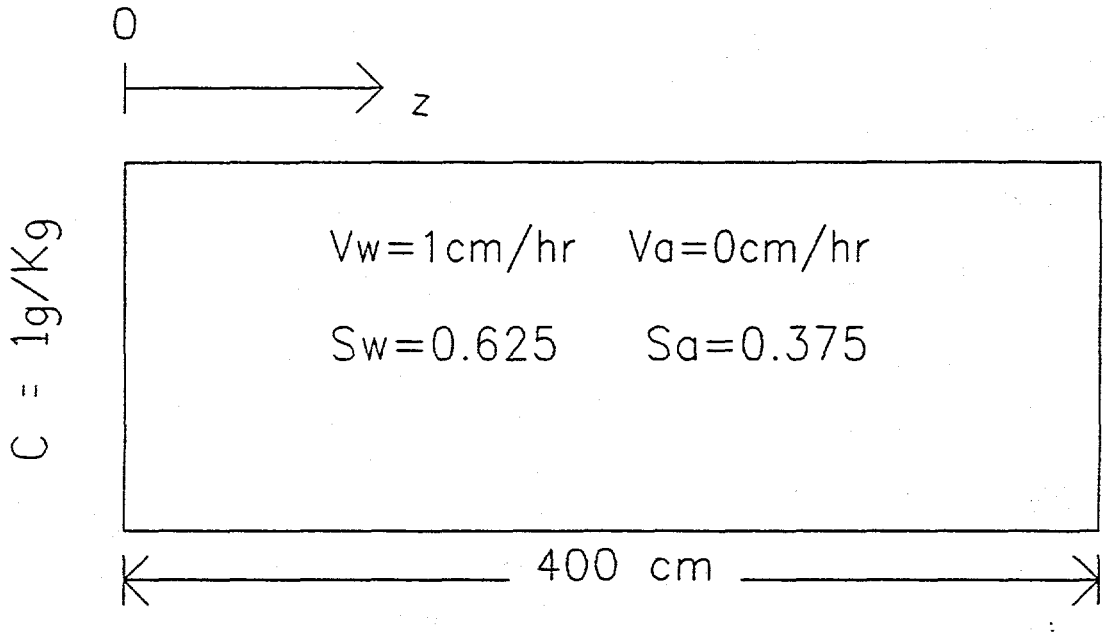


Figure 4.30 Schematic diagram for the example in 4.5.1.1.

Table 4.13 Simulation data for the semi-infinite soil column example.

PARAMETER	VALUE
Effective porosity, ϕ	0.4
Water density, ρ_w	1.0 g/cm^3
LNAPL density, ρ_n	0.95 g/cm^3
Air density, ρ_a	0.001 g/cm^3
Distribution coefficient, k_d	0.0
Partitioning coefficient, κ_n	0.0
Henry's constant, κ_a	0.0
Decay coefficient, λ	0.0
Longitudinal dispersivity, α_L	5.0 cm
Water diffusion coefficient, D_{mw}	0.0
NAPL diffusion coefficient, D_{mn}	0.0
Air diffusion coefficient, D_{ma}	0.0
Water saturation, S_w	0.625
NAPL saturation, S_n	0.375
Air saturation, S_a	0.0
Water Darcy velocity, V_w	1.0 cm/hr
NAPL Darcy velocity, V_n	0.0
Air Darcy velocity, V_a	0.0
Δz	10.0 cm
Δt	0.5 hr

The numerical solution obtained from the SAMFT1D code was checked against the analytical solution of Ogata and Banks (1961). Shown in Figure 4.31 are the concentration profiles at 25 and 50 hours from the simulation. As can be seen, the numerical and analytical solutions are in good agreement.

4.5.1.2 Solute Transport in a Finite Soil Column

In this problem, downward vertical transport of a dissolved contaminant is examined in a 20 m long unsaturated soil column. The water saturation in the system is fixed at 0.625. Again, all partition coefficients are assumed to be zero. The schematic description of the example is given in Figure 4.32. The initial solute concentration in the soil column is assumed to be zero and the solute is injected into the column from the inlet section at a prescribed solute mass flux. The complete listing of values of physical parameters and discretization data used in the numerical simulation is given in Table 4.14.

Results for 5, 10 and 20 days obtained from the SAMFT1D code are compared in Figure 4.33 with the analytical solution given by van Genuchten and Alves (1982). There is good agreement between the numerical and analytical solutions.

4.5.2 Three-Phase Examples: One-Dimensional Transport of Dissolved Mass of LNAPL Spill

In this section, the solute transport part of the SAMFT1D code is tested against a realistic multiphase solute transport scenario. This example is a continuation of the multiphase flow problem presented in Section 4.4.7, and was selected to demonstrate an application of

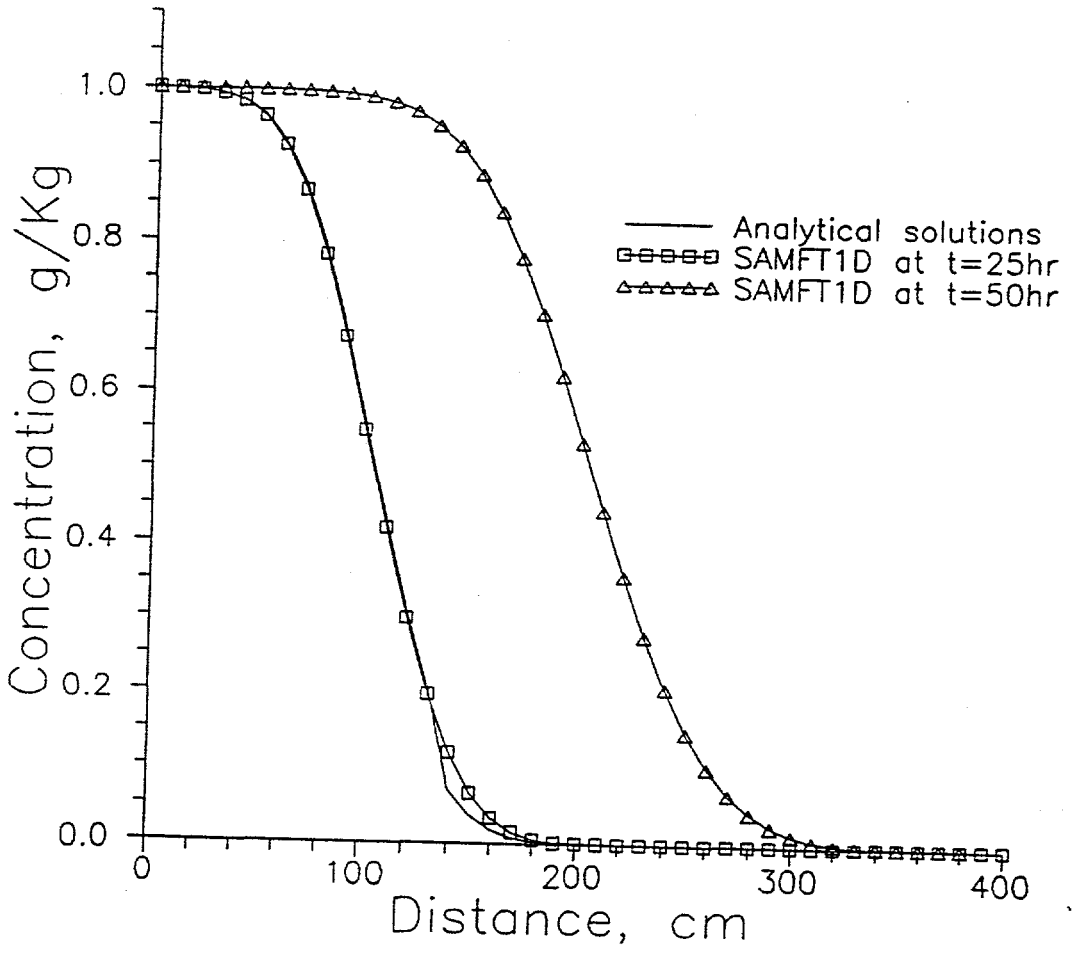


Figure 4.31 Concentration profiles for the example in 4.5.1.1.

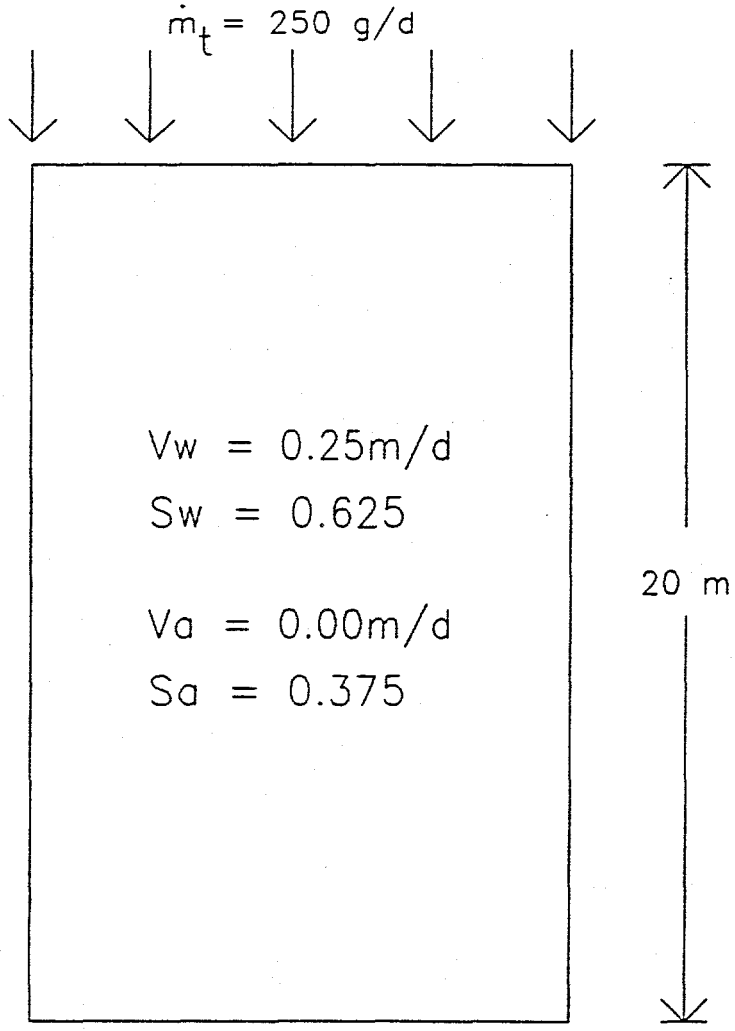


Figure 4.32 Schematic diagram for the example in 4.5.1.2.

Table 4.14 Simulation data for the finite soil column example.

PARAMETER	VALUE
Effective porosity, ϕ	0.4
Water density, ρ_w	1000 kg/m^3
LNAPL density, ρ_n	950 kg/m^3
Air density, ρ_a	1.0 kg/m^3
Distribution coefficient, k_d	0.0
Partitioning coefficient, κ_n	0.0
Henry's constant, κ_a	0.0
Decay coefficient, λ	0.0
Longitudinal dispersivity, α_L	4.0 cm
Water diffusion coefficient, D_{mw}	0.0
NAPL diffusion coefficient, D_{mn}	0.0
Air diffusion coefficient, D_{ma}	0.0
Water saturation, S_w	0.625
NAPL saturation, S_n	0.375
Air saturation, S_a	0.0
Water Darcy velocity, V_w	0.25 m/d
NAPL Darcy velocity, V_n	0.0
Air Darcy velocity, V_a	0.0
Δz	1.0 m
Δt	0.5 d

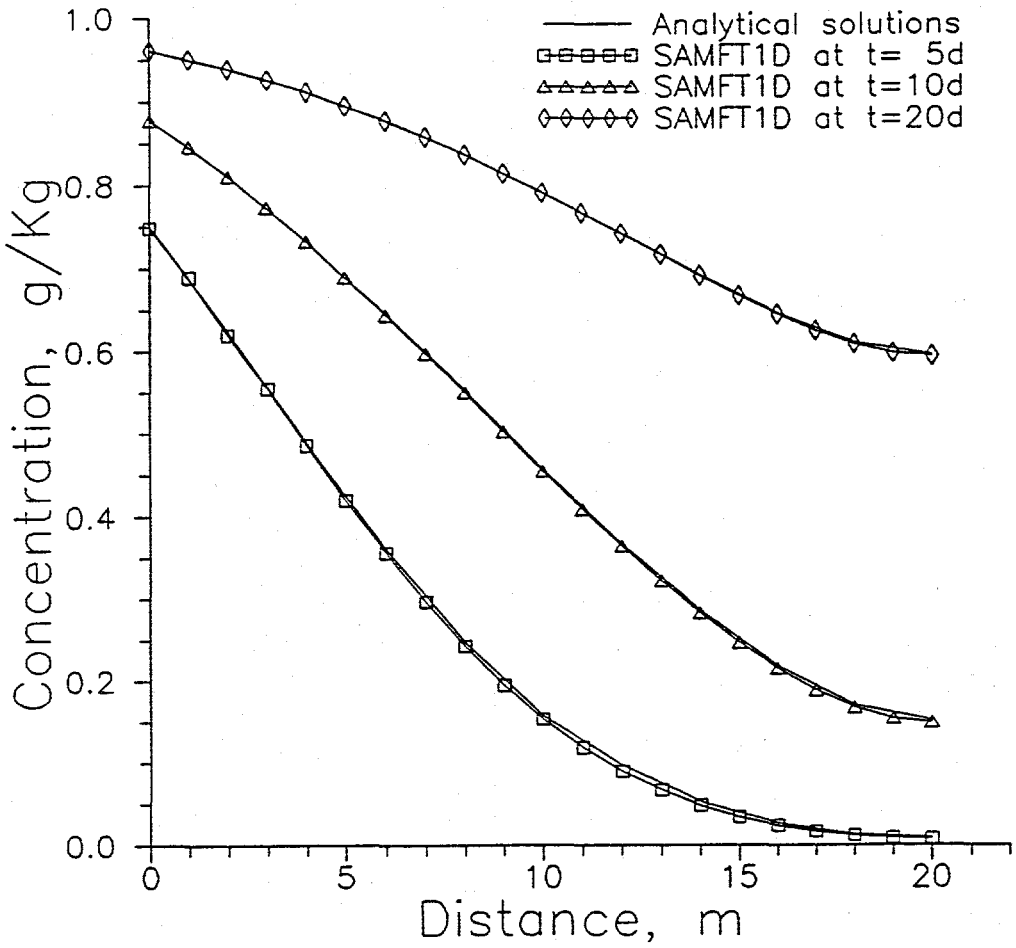


Figure 4.33 Concentration profiles for the example in 4.5.1.2.

SAMFT2D to a more complex problem involving a pulse release of single-component LNAPL mass that was captured within the unsaturated zone by capillary forces and subsequently transported to the water table by dissolution. This is a typical situation when an accidental spill of LNAPL on the ground surface provides a discontinuous contaminant source. To handle this situation, both three-phase flow and single-component transport simulations were performed. The fluid phase saturation and velocity distributions determined from the flow simulation were used as input for the transport simulation.

The flow domain and boundary conditions are depicted in Figure 4.28. The domain was discretized using a grid consisting of 20 elements with constant nodal spacings ($\Delta z = 0.50$ m). The surface boundary was subjected to water and LNAPL injection from $t = 0$. After 75 days, the LNAPL injection stopped, the water injection continued, and the air pressure was kept atmospheric. For this flow simulation, we used the same data for soil and fluid properties, relative permeability and capillary pressure as given for the flow problem in Section 4.4.7. The initial condition data was generated by the code with zero flux value for water and NAPL and $P_a = P_{atm}$ on the top boundary. Time stepping was performed until the LNAPL mass became completely immobile. The steady-state profile of LNAPL saturation, which was reached at $t =$ 500 days is depicted in Figure 4.29.

Following the flow simulation, two single-component transport simulations were performed. In the first case, the stagnant NAPL mass is assumed to be one-component contaminant. The pure NAPL is regarded as the precipitated phase and its mass treated as "precipitated mass (see Section 2.3.2)". In the second case, the NAPL mass is assumed to be composed of multiple components and we are interested in the transport of a single soluble

volatile organic component. In both cases, temporal and spatial distributions of contaminant in the system are observed when freshwater injection is kept steady at the inflow boundary as in the flow simulation.

4.5.2.1 One-Component NAPL Mass Regarded as Precipitated Mass

The single-component LNAPL was assumed to be lightly soluble in water and air. A schematic description of the transport problem is shown in Figure 4.34. The transport parameter values used are listed in Table 4.15. The initial condition of the transport problem corresponds to the steady-state condition of the flow problem.

Note that since the LNAPL mass was treated as the precipitated mass, contributions from the LNAPL phase transport were effectively "turned off" by setting $\kappa_n = 0$. The simulation was performed for approximately 6.3 years. In Figure 4.35, profiles of concentrations in various phases (water, air and solid) are presented at time values of 1.5 and 6.3 years. The maximum concentration values were predicted by the model in the upper portion of the domain where the LNAPL mass existed. Furthermore, the buildup of concentration profiles with time was due to dissolution of the immobile LNAPL mass. Shown in Figure 4.36 are the contaminant mass distributions in all four phases. The curves clearly show the reduction of mass of the stagnant LNAPL and the increases in the soluble-component masses in the other phases. Note that for $t = 6.3$ years, the contaminant mass curves for the water and air phases show abrupt increase and decrease in the contaminant mass near the end of the domain (adjacent to the water table). This is due to the abrupt increase and decrease in water-phase and air-phase saturations in that part of the domain.

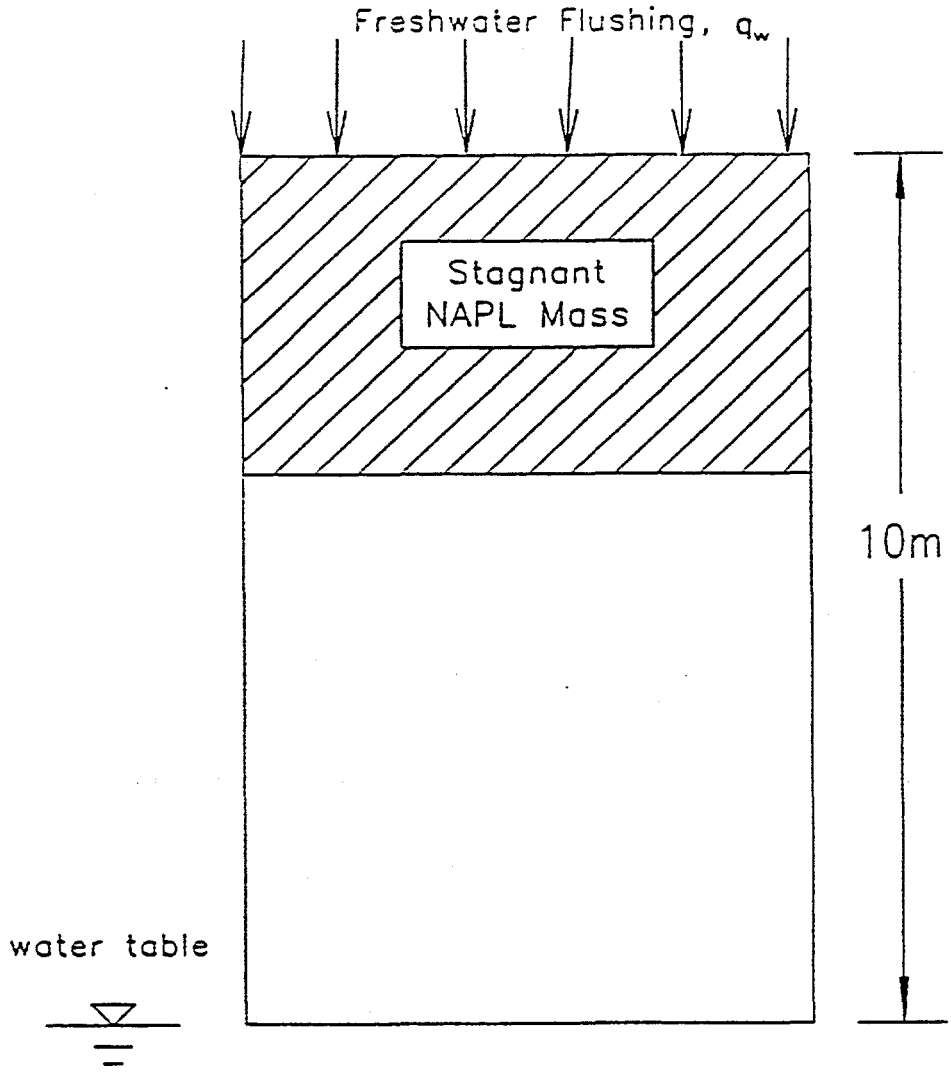


Figure 4.34 Schematic diagram for the example in 4.5.2.1.

Table 4.15 Simulation data for the precipitated mass transport problem.

PARAMETER	VALUE
Effective porosity, ϕ	0.3
Water density, ρ_w	1000 kg/m^3
LNAPL density, ρ_n	950 kg/m^3
Air density, ρ_a	1.18 kg/m^3
Soil bulk density, ρ_B	1500 kg/m^3
Distribution coefficient, k_d	0.0001 m^3/kg
Water solubility, c_{ws}	0.01
Henry's constant, κ_a	0.25
Decay coefficient, λ	0.0
Longitudinal dispersivity, α_L	1.0 m
Tortuosity, τ	0.58
Exponent, n	3.3
Water diffusion coefficient, D_{mw}	8.64×10^{-5} m^2/d
Air diffusion coefficient, D_{ma}	0.864 m^2/d
Δz	0.5 m
Δt	57.9 d

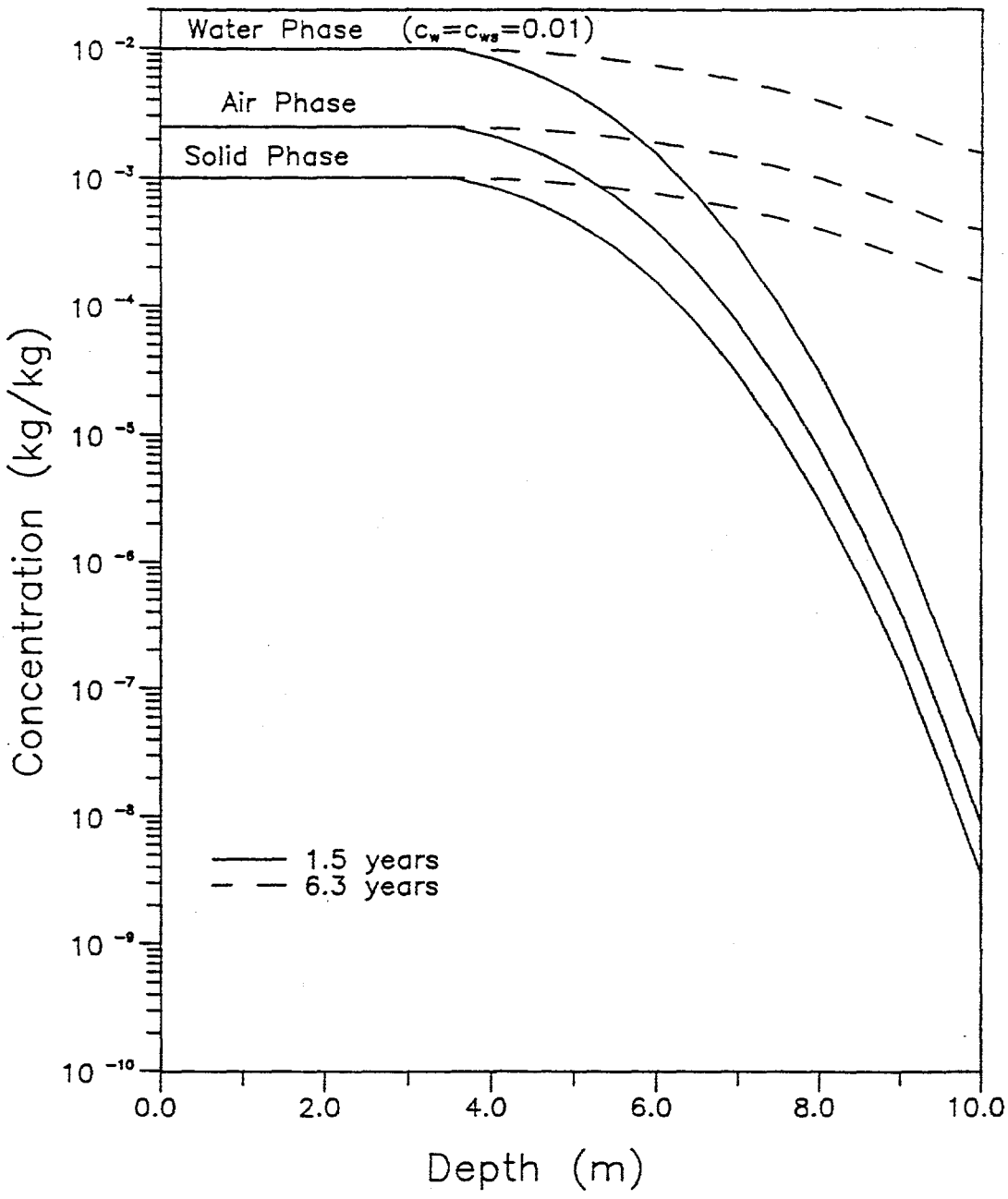


Figure 4.35 Concentration profiles for the example in 4.5.2.1.

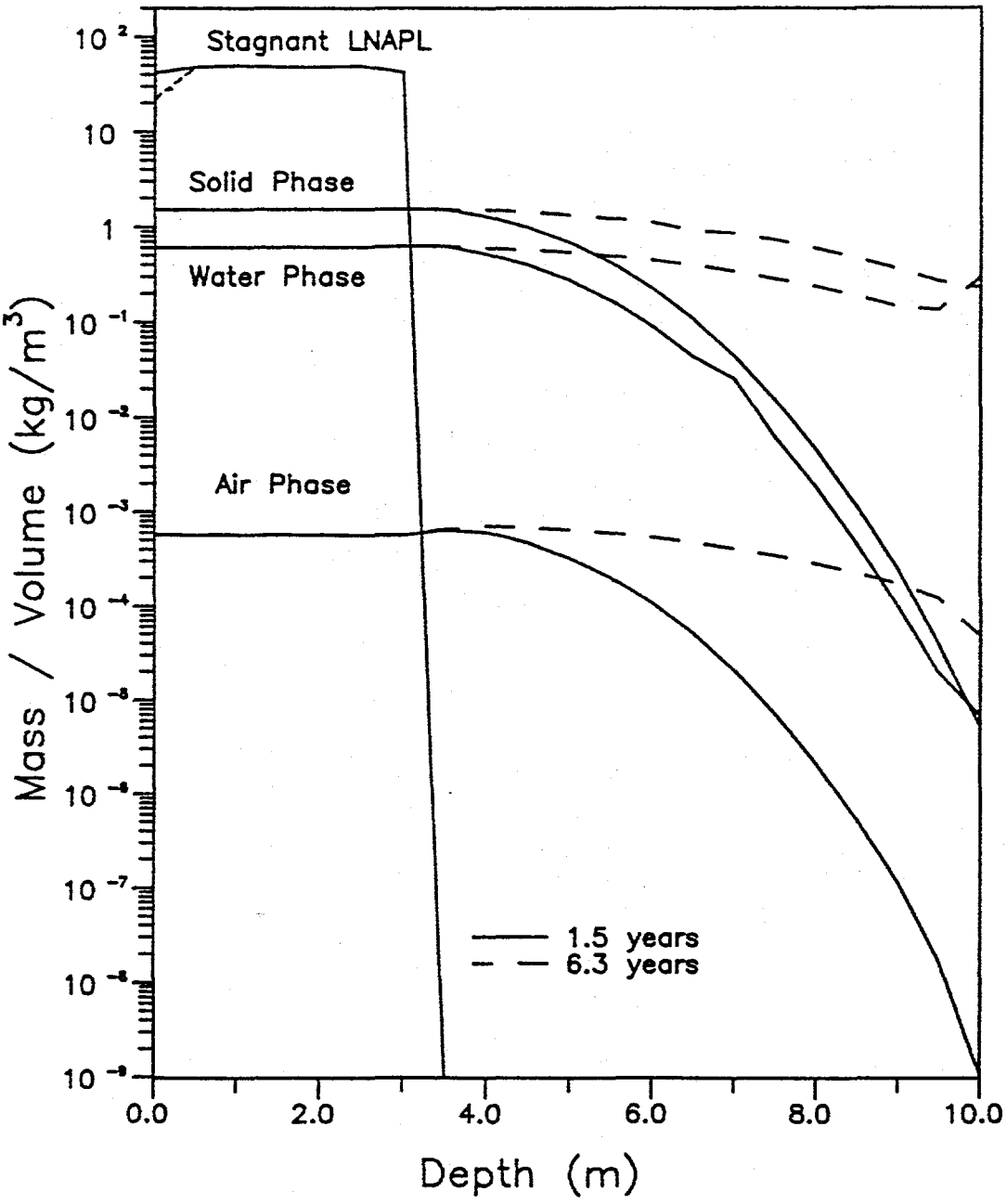


Figure 4.36 Distribution of mass for the example in 4.5.2.1.

4.5.2.2 Single Component Contaminant in Multi-Component NAPL Mass

In this case, the stagnant NAPL mass is composed of multiple soluble components and we are interested in the fate of a component whose mass fraction is 2.5% of the entire NAPL mass. The dissolved component concentration is assumed to be well below the solubility limit. All parameters are identical to the first case except for those noted in Table 4.16.

Since there is no precipitation of the component concerned, we can expect immediate reduction in the concentration values in the part of the domain where the NAPL was initially present. See Figures 4.37 and 4.38 for the soluble-component concentration and mass distributions, respectively, at different time levels. It may be noted that the soluble-component concentration diminishes in the lower portion of the domain where the NAPL is absent.

Table 4.16 Simulation data for the non-precipitated mass transport problem.

PARAMETER	VALUE
Distribution coefficient, k_d	0.00015 m^3/kg
Partitioning coefficient, κ_n	0.01
Henry's constant, κ_a	0.10

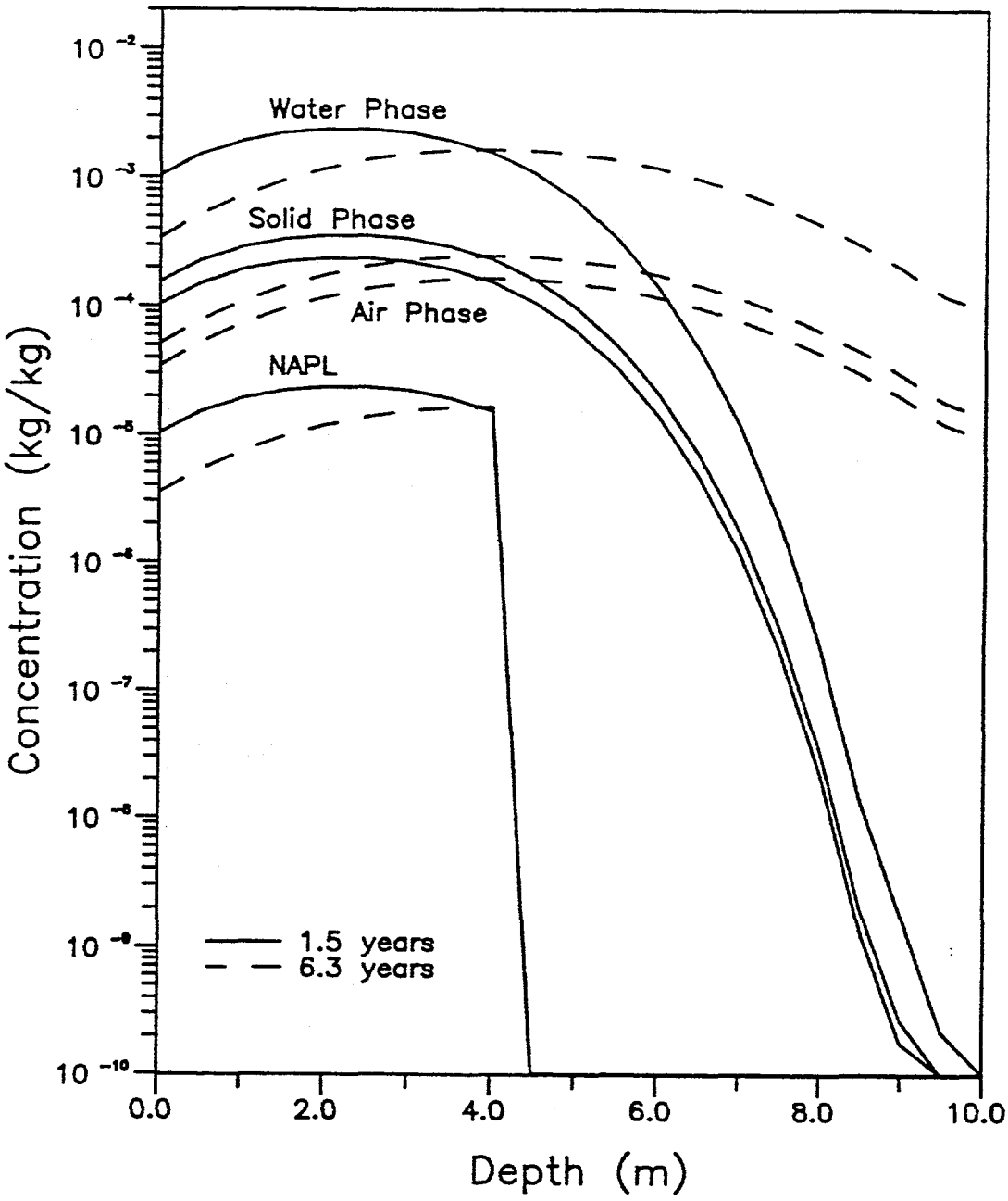


Figure 4.37 Concentration profiles for the example in 4.5.2.2.

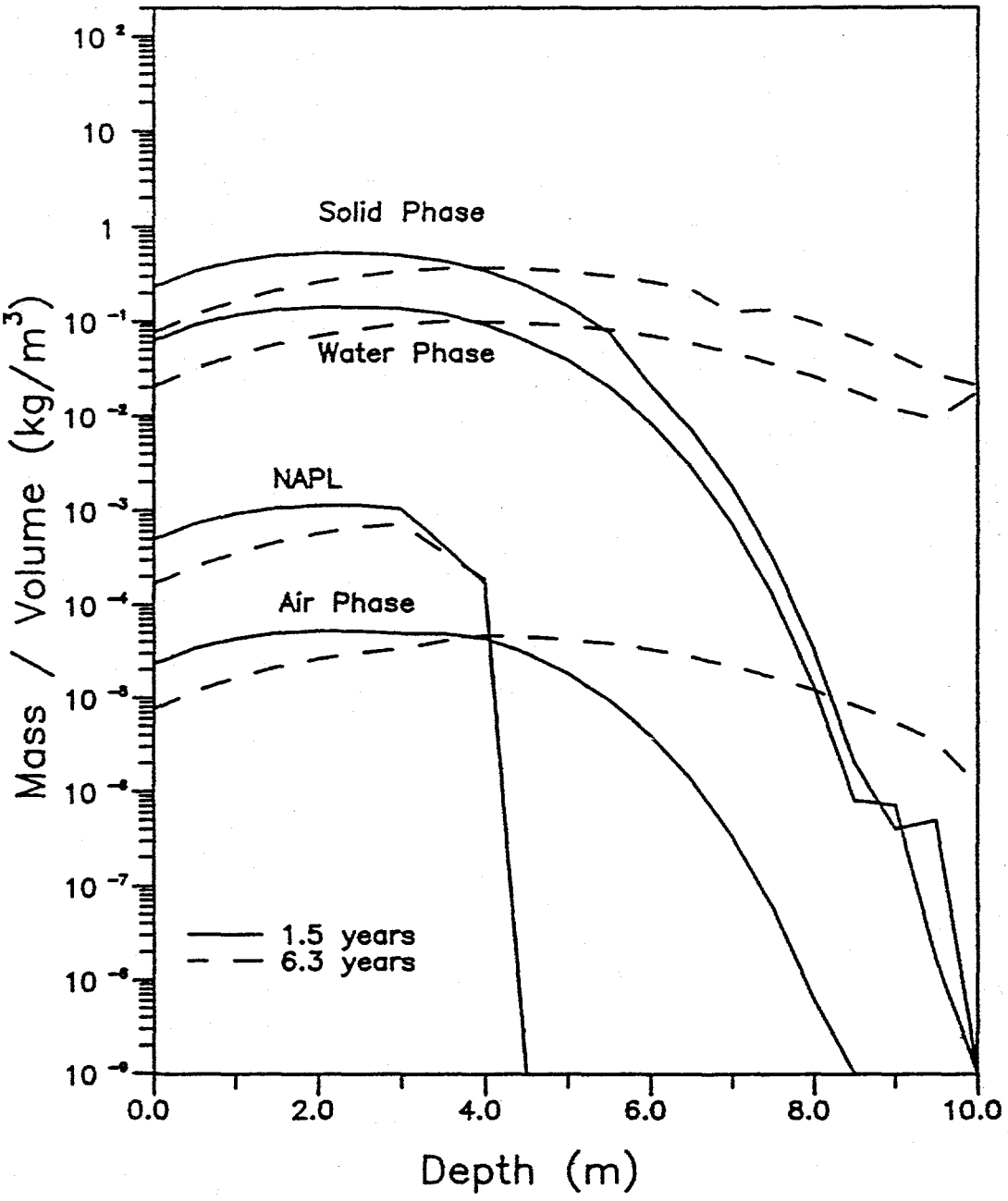


Figure 4.38 Distribution of mass for the example in 4.5.2.2.

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5 PROBLEM DEFINITION AND SIMULATION PROCEDURE

5.1 TYPES OF PROBLEMS

The SAMFT1D code can be used in several types of investigations of fluid flow and contaminant transport in the subsurface. For demonstrative purposes, two typical examples are described. The first example (Figure 5.1) concerns the assessment of leachate migration via the unsaturated zone to the water table of an unconfined aquifer system. For the depicted situation, SAMFT1D may be used to simulate one-dimensional infiltration and transport in the unsaturated zone directly beneath the land disposal unit. Output of water and contaminant fluxes at the water table may be used in a preliminary risk assessment or a multi-dimensional analysis of flow and transport in the saturated zone.

The second example (Figure 5.2) concerns the assessment of NAPL movement in the unsaturated zone. For the depicted situation, SAMFT1D may be used to simulate two-phase or three-phase flow and determine whether the NAPL mass is released from the source (e.g., a leaky underground storage tank or an accidental spill) will reach the water table.

5.2 DATA REQUIREMENTS

Data required for the simulation of variably saturated, single-phase or multiphase flow include intrinsic permeability and compressibility of the porous medium, fluid properties, the geometry and configuration of the flow region, as well as initial and boundary conditions of the problem. Additionally, data pertaining to fluid retention characteristics and relative permeability of the porous medium needs to be supplied to the code either in a functional form or tabulation.

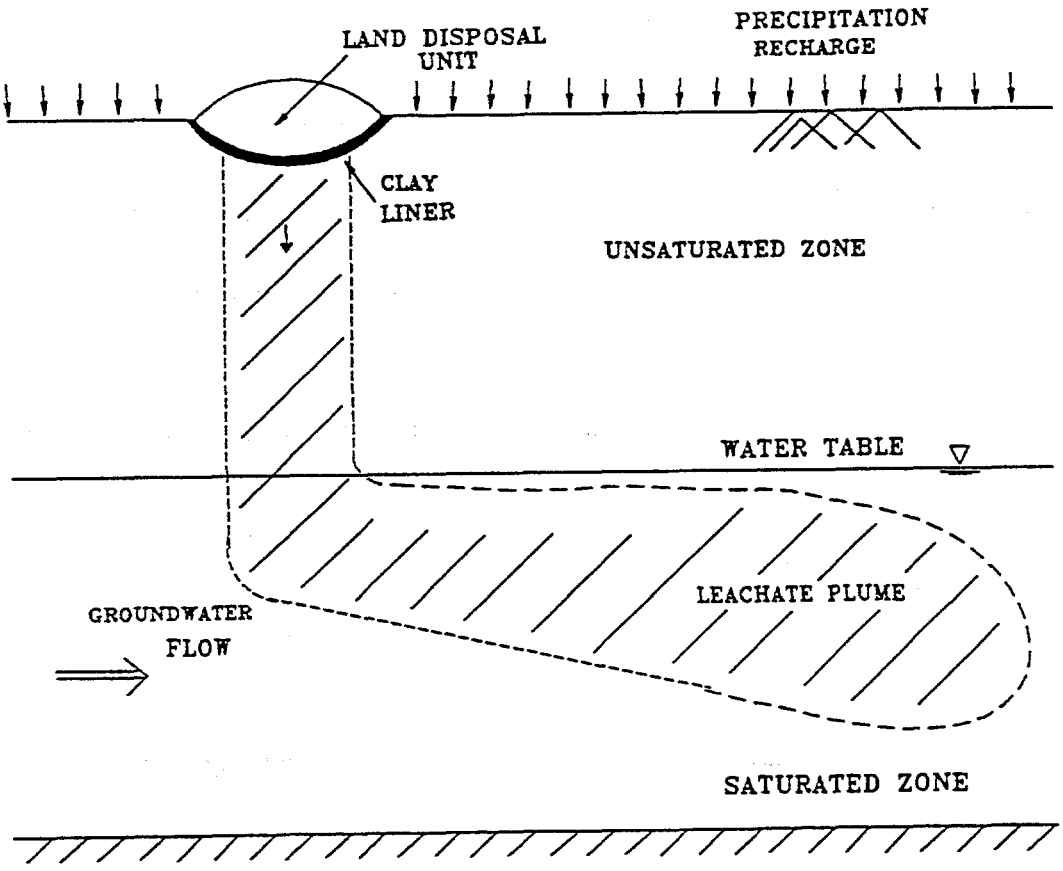

Figure 5.1 Moisture movement and leachate migration in the unsaturated zone.

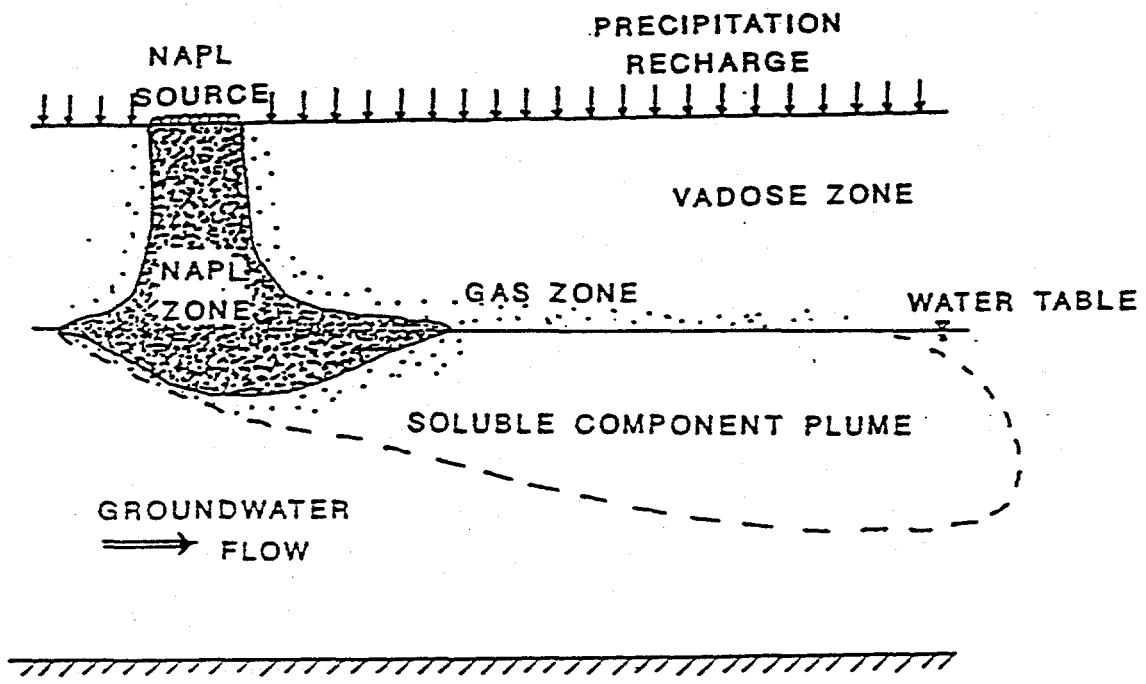

Figure 5.2 NAPL transport in the unsaturated zone.

Data required for the simulation of solute transport includes longitudinal dispersivity of the porous media, solute properties (i.e., distribution, decay and partitioning coefficients), as well as contaminant source characteristics (source location, geometry, concentration, and fluxes), Darcy velocity and saturation of each active fluid phase, and initial and boundary conditions associated with the single-species transport problem.

5.3 SIMULATION PROCEDURE

The general procedure for using SAMFT1D to simulate fluid flow and/or solute transport in subsurface systems is outlined below.

- Prepare a diagrammatic description of the problem such as those shown in Figures 5.1 and 5.2. The diagram should depict the solution region together with a description of the zones of different material properties and boundary conditions.

- Prepare a list of material numbers and properties to be supplied to the code.

- Prepare steady-state boundary condition data. These data are classified into two sets. The first set consists of global node numbers and prescribed values of dependent variables to be determined. The second set consists of global node numbers and prescribed values of integrated nodal fluxes. If there are no steady-state boundary conditions, this step of the simulation procedure may be omitted.

- Prepare transient boundary condition data. The data are also classified into two sets. The first set consists of global node numbers and the time graph of prescribed values of dependent variables to be determined. The second set consists of global node numbers and the time graph of prescribed values of integrated nodal fluxes.

- Follow the input data preparation instructions given in Chapter 8 and supply the required input to the code.

- Run the code and interpret the output using the guide provided in Chapter 9.

5.4 GRID SPECIFICATION

A mesh-centered, finite element grid is used by the code to handle single-phase flow and single- and multiple-phase transport problems. The number of nodes in the grid equals the number of linear elements plus one. A block-centered, finite difference grid is used to handle multiphase flow problems. If dealing with combined multiphase flow and transport simulations, the block-centered grid should be used by the user, and the code will generate internally a mesh-center grid for the transport runs. The number of nodes in the block-centered grid is equal to the number of grid blocks. Grid generation is performed automatically by the code. In each case, the user needs to specify the following input parameters:

Record group 11 (see Section 8.3)

NLAYER: Number of layers or zones to be discretized.

IBCGR: Grid type identifier,
= 0 for finite element,
= 1 for block-centered finite difference.

ACROS: Cross-sectional area of the flow domain.

IHORGR: Grid orientation identifier,
= 0 for vertical,
= 1 for horizontal.

Record group 12

Number of records = NLAYER.

ILAYR: Layer or zone number.

NELM(ILAYR): Number of elements or grid blocks in layer ILAYR.

IMATL(ILAYR): Material number for the layer.

THL (ILAYR): Layer thickness.

Nodes and elements are numbered sequentially from left to right for a horizontal grid and from top to bottom of the flow domain for a vertical grid.

5.5 INITIAL AND BOUNDARY CONDITION SPECIFICATIONS

5.5.1 Single-Phase Flow and Transport Modeling

To perform a transient flow or transport analysis or a steady-state flow analysis, an initial distribution of each primary dependent variable to be solved must be applied to the code. If the initial distribution is uniform, it is sufficient to supply constant default values to the code.

In a fluid flow simulation, a default nonuniform initial condition may also be specified to the code by means of an initial function option (see record group 7 in Section 8.3 of Chapter 8).

For a general case of nonuniform initial distribution, it is necessary to supply initial nodal values to the code. The number of nodes where initial values differ from the default value (NPIN) may be less than or equal to the total number of nodes (NP). The input initial values are used by the code to override the default values.

Boundary conditions can be given in terms of either the Dirichlet prescribed values of the dependent variables, or in terms of the fluid or solute flux at boundary nodes. Specification of a Dirichlet first-type boundary condition is very straightforward and requires no further explanation. Specifying the nodal boundary condition value in the case of a flux-type boundary condition is described below.

For a fluid flow analysis, the fluid flux at a node corresponds to the mass flow rate of the concerned fluid per unit cross-sectional area. The sign convention for flux adopted by the code is positive for influx and negative for efflux.

For a solute transport analysis, the solute flux at a node corresponds to the rate of solute mass entering the node per unit cross-sectional area.

Steady-state boundary conditions are handled simply by specifying the node numbers and prescribed values of the dependent variables or mass fluxes of fluid or solute. Transient boundary conditions are also handled in a convenient manner by specifying the node numbers and relationships of time versus the prescribed values. The code admits both continuous and stepped temporal variations (Figure 5.3). A continuous variation is represented using the piecewise linear approximation passing through a number of control points. A discontinuous variation is represented using a stepped approximation passing through control points. The total number of control points is equal to the number of steps plus one.

5.5.2 Multiphase Flow and Transport Modeling

In a multiphase flow simulation, the undisturbed initial condition of the multiphase system is considered to be at equilibrium between capillary pressure and gravity in SAMFT1D. The code provides three options for initialization of the default initial conditions using three dependent variables, P_w, S_w and S_n supplied by the user, based on the assumption that the initial saturation (S_{no}) of the second fluid phase (NAPL) and the initial pressure (P_{atm}) of the third phase (air) are constants, (see record group 7 in Section 8.3 of Chapter 8). The equations used

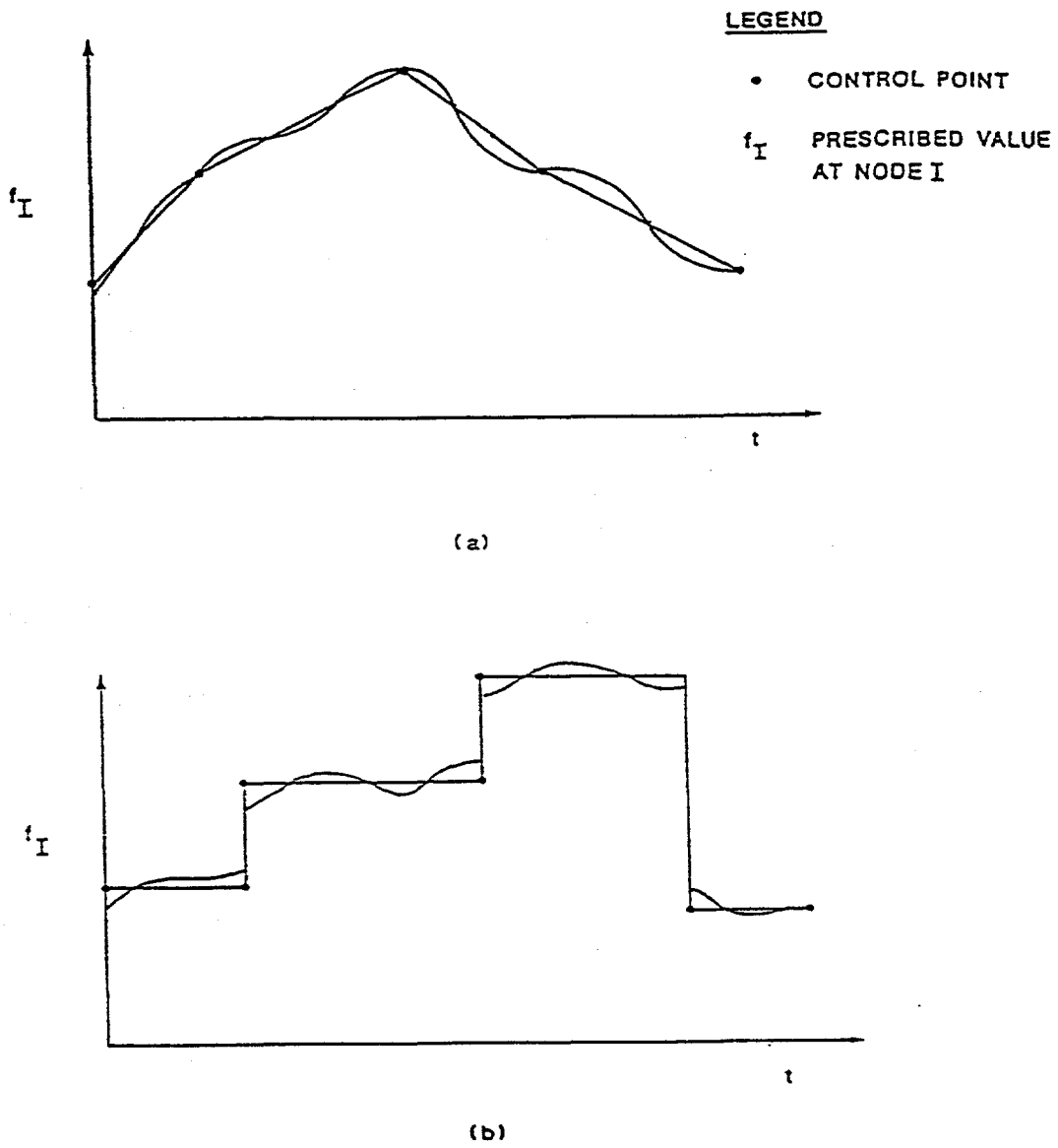

Figure 5.3 Modeled approximations for continuous and discontinuous variations of prescribed function at node I.

in the code to determine the default initial conditions of the primary variables for flow simulations are discussed in Section 3.3.1.3.

For a general case of nonuniform initial conditions, it is necessary to input all the initial nodal values for the code. The number of nodes whose initial values differ from the default values (NPIN) may be equal to or smaller than the total number of nodes. The input initial values are used by the code to override the default values.

Boundary conditions can be provided either in terms of the prescribed pressure values, or in terms of the fluid flux values. The treatment of boundary conditions for multiphase flow is a more complicated than that for single phase flow, discussed in the previous section. It is necessary to distinguish if the boundary condition is that of injection or production in order that the correct source or sink terms may be calculated for the boundary nodes. For injection flux boundary condition, the inflow rate for each phase should be specified separately. When one deals with flux specified production or sink nodes, only total liquid production rate needs to be input. For pressure injection boundary conditions, the code generates a source term only for phase ℓ (ℓ=w, n or a) if P_ℓ is specified. In the case of production boundary pressure, P^B is proposed, the code will set that $P_\ell = P^B$ for each phase ℓ, and no fluids will be allowed to flow back into the boundary nodes.

For a solute transport analysis in a multiple fluid system, the treatment and specification of the boundary and initial condition are similar to those in a single-phase transport problem. However, there are certain differences in the initial condition specification and flux boundary condition description. Since the multiphase transport modules of SAMFT1D take into account the solubility limit of the solute in water phase, the initial precipitated solute mass distribution

should be supplied to the code. For convenience, the flux boundary conditions in multiphase transport problems are treated in terms of partitioned fluid mass and total solute mass flux, as discussed in Sections 2.3.2 and 8.2, respectively.

6 CODE STRUCTURE

6.1 CODE ORGANIZATION AND MODULE DESCRIPTION

The SAMFT1D code is structured to accommodate two sets of computational modules designed to perform single-phase and multiphase analyses, respectively, which are described herein.

Shown in Figure 6.1 is a schematic flow chart depicting major computational steps for single-phase, variably saturated flow and transport analysis. Note that three modeling options (IMODL=1, 0 and 2) are provided. With these options, the user may instruct the code to perform: single or multiphase flow simulation only, solute transport simulation or dual simulation of flow and transport. A grid consisting of linear one-dimensional elements is generated and used by the code to represent the region of interest. The solutions of the tridiagonal matrix equations resulting from finite element discretizations of the single-phase flow and transport equations are performed using the Thomas algorithm. Nonlinear treatment of the variably saturated flow problem is performed using the Newton-Raphson scheme described in Chapter 3.

The code structure for the multiphase flow modules is similar to that for the single-phase flow ones, and the major computational procedures are shown in Figure 6.2. A block-centered grid is generated and used to describe a one-dimensional multiphase flow problem employing the finite difference scheme. The resulting non-linear algebraic finite difference equations are solved fully implicitly by the Newton-Raphson method. The fully upstream weighting technique

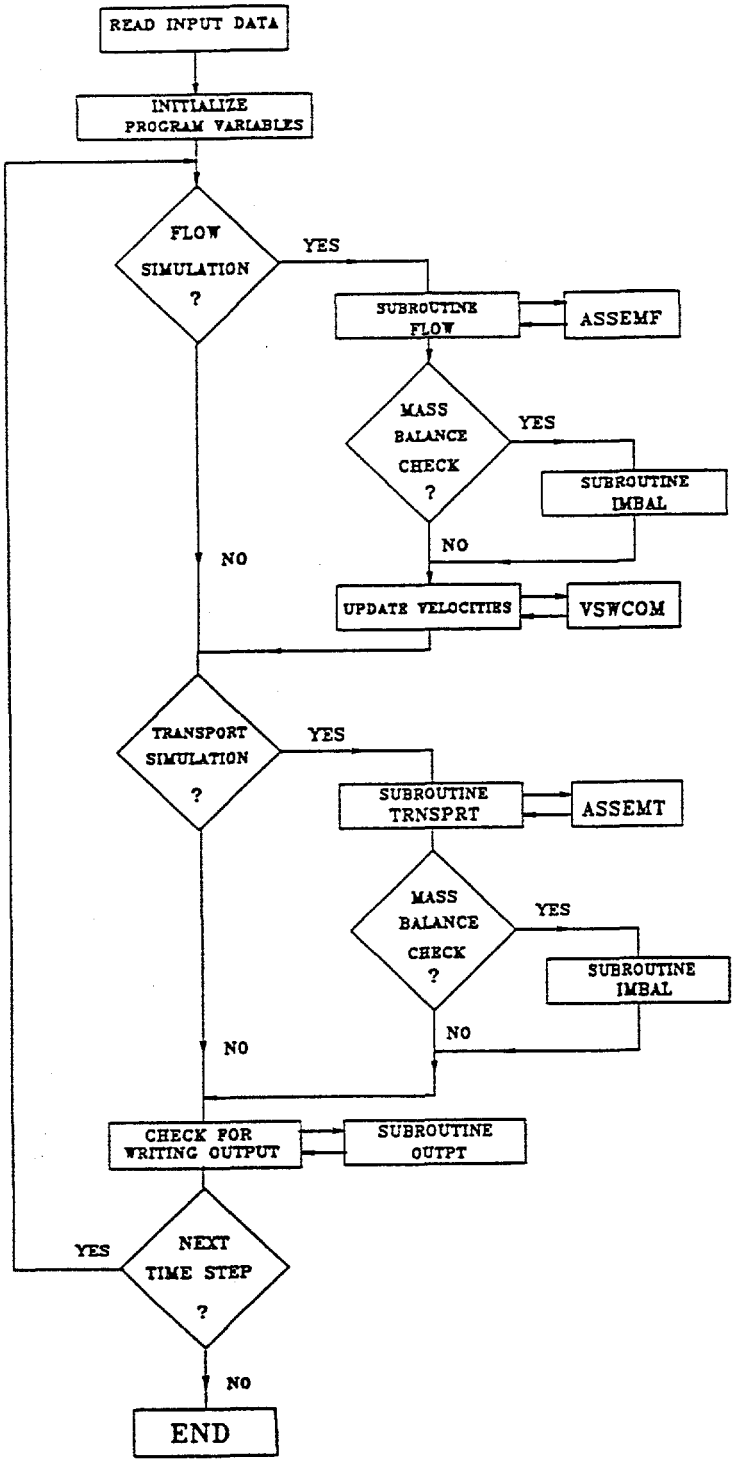

Figure 6.1 Flowchart for the single phase flow and transport modules of SAMFT1D.

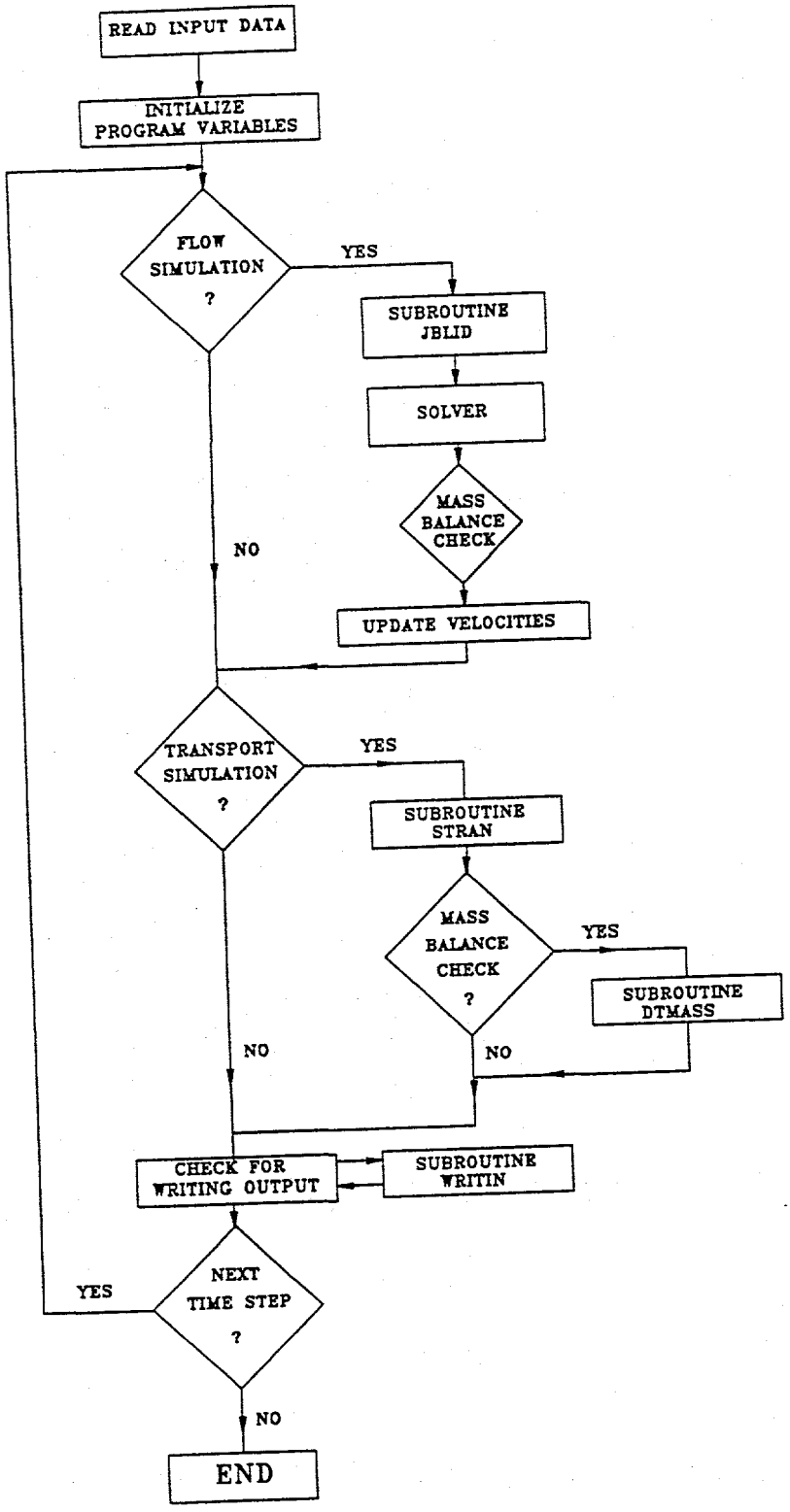

Figure 6.2 Flowchart for the multiphase flow and transport modules of SAMFT1D.

is employed to evaluate inter-grid-block mobility values. An option of mass balance computation is available for both flow and transport analyses in the single- or multiple-phase modules.

6.2 INTERNAL DATA STRUCTURE

Data necessary for the finite element or finite difference analysis performed by the code is classified according to single-phase or multiphase flow and transport analysis as follows:

The internal data structure for multiphase flow analyses parallels that for the single phase modules.

For a single-phase and transport analysis:

(1) Material properties. The material properties of soils and fluids pertaining to single phase flow and transport analyses are stored in array form in common blocks labeled FSDATA, CTRANS and FSDATA, respectively. Inside the computational routines, the data are transferred to common blocks MDATA and SWHDA.

(2) Mesh data and element material numbers. Data related to the linear finite element discretization of the one-dimensional domain is stored in common blocks, AELEM, MSHDAT and ESTORE.

(3) Boundary condition data. Either steady state or transient boundary conditions may be prescribed. The number of applicable boundary conditions are stored in common block CNTRBC. Steady state Dirichlet and flux conditions are stored in common blocks labeled BCDATA and BCDATC. Time dependent boundary conditions are stored in common blocks BCDATC and BCDATD.

(4) Initial condition data and computed nodal values of the dependent variables.

These data are read in and stored in two common blocks INDATA and WAVE1. The secondary variables (velocities, saturations) are stored in the common block VELEM.

(5) Control parameters. Simulation control parameters are stored in common blocks CONTR1 and CONTR3. In the computational routines for single phase flow and transport, the relevant parameters are transferred to common block CONTR.

(6) Time discretization and output specification data. The related parameters are stored in common blocks TIMDAT and TOUT.

(7) Observation node data. Parameters related to nodes that are identified as observation nodes, as well as computed values of primary variables at these nodes are stored in common block OBSERV.

For the multiphase flow and transport analysis:

(1) Material properties. The material properties of soils and fluids pertaining to multiphase flow and transport analyses are read in and stored in three common blocks labeled KRPC, FSDATA and CTRANS, respectively.

(2) Mesh data and element material numbers. For the block-centered mesh data generated by the code, the layers and element material numbers are stored in three common blocks labeled MSHDAT, AELEM and GDATA, respectively.

(3) Boundary condition data. Steady-state Dirichlet and prescribed flux conditions are read in and stored in two common blocks labeled BCDATA and BCDATB. The block BCDATA contains arrays that store node numbers and prescribed pressure values. The block BCDATB contains arrays that store node numbers and values of nodal fluxes. Transient Dirichlet and prescribed flux conditions are read in and stored in a common block labeled

BCDATC. This block also contains arrays that store numbers of control points on the time graph of the pressure or flux boundary conditions.

(4) Initial condition data and computed nodal values of the dependent variables. These are stored in three common blocks labeled INDATA, PRIMVS, and CTRANS, respectively.

(5) Element geometrical and storage properties. These are stored in a common block labeled ESTORE.

(6) Element Darcy velocities and phase saturations. These are stored in two common blocks labeled VSPDAT, and DVELF, respectively.

(7) Control parameters. Various control parameters of the problem and simulation are stored in five common blocks labeled CONTR1, CONTR3, CONTRC, CNTRBC, and IDRUN.

(8) Time discretization and output specification data. These are stored in two common blocks labeled TIMDAT, and TOUT, respectively.

(9) Observation mode data. Parameters related to nodes that are identified as observation nodes, as well as computed values of primary variables at these nodes are stored in common block OBSERV.

6.3 DIMENSION LIMITS

No dynamic dimensioning is employed in the code. All of the important arrays are stored in labeled common blocks. The dimension limits of the principal arrays are summarized below. These must be observed by the user when applying the code to practical problems.

Maximum total number of nodal points	= 201
Maximum total number of elements	= 200
Maximum number of time steps	= 200
Maximum number of different sets of material properties	= 20
Maximum number of data points in defining constitutive relations	= 30
Maximum number of steady-state Dirichlet boundary conditions	= 50
Maximum number of steady-state flux boundary conditions	= 50
Maximum number of time-dependent, Dirichlet boundary nodes	= 50
Maximum number of time-dependent, flux boundary nodes	= 50
Maximum number of nodes for which flux computation is required	= 50
Maximum number of observation nodes	= 50
Maximum number of time values for transient boundary conditions	= 50

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7 DATA FILES

7.1 MAIN INPUT AND OUTPUT FILES

There are two major input and output files used by the SAMFT1D code on units 5 and 6, respectively. These files are described as follows:

1. File number 5. This is the input file containing the essential input data for each run of the code. The content of this file as well as the description of input variables are provided in Section 8.3 of Chapter 8.

2. File number 6. This is the output file containing the line printer output from the code. The content of this file as well as the description of output variables are provided in Chapter 9.

In addition to the major files on units 5 and 6, several backup files may be needed by the code to perform a restart run or, two consecutive runs of flow and related transport problems, and to create output for plotting purposes.

7.2 BACKUP FILES

There are 4 backup files that may be used by the code, which are written on units 8, 9, 10, and 11. These files are described below.

1. File number 8. This is the backup output file containing nodal values of the primary dependent variables that were computed at the final time step of the current run. Information in this file can be used as the initial conditions for the next restart run. File number

8 is written only when the control input variable NOWRIT is set equal to 1. The file contains the following information corresponding to the end of the final time step:

- Title heading giving final time value.
- List of nodal values of the primary dependent variables (fluid pressure and saturation or concentration, depending on whether one is dealing with flow or transport) at the final time level. These nodal values are written in the FORMAT (6E16.4).

The set of nodal values written on file unit 8 can be used as an initial condition for the restart run of a given problem. To do this, the user needs either to read unit 8 directly by set NONU=2 or to delete the heading record of the file on unit 8 and assemble this file as part of the input file on unit 5 (see Section 8.3 for the input preparation guide).

2. File number 9. This backup file is written when the flow simulation is performed and the value of the output control parameter NVWRIT is greater than 0. For each specified time level of the flow simulation, this output file on unit 9 contains the following information:

- Title heading, giving the time value.
- List of element centroidal values of Darcy velocity components for each active fluid phase. For multiphase flow problems, phase saturations of all the phases are also included.
- List of storage capacity values at the nodes for single-phase analysis. This information is written only when the mass balance calculation option, IMBAL, is set equal to 1.

The output file on unit 9 from the flow simulation can be used as backup input for the subsequent and related transport simulation. To do this, the user should proceed by editing the input file on unit 5 as follows:

- Set the control parameter NVREAD (see record group 5 in Sections 8.3) equal to 1. This directs the code to read velocity data from the file on unit 9.

3. File number 10. This file is written when the value of the plotting control parameter NPLOT of record group 5 is greater than zero.

For NPLOT=n, the output file on unit 10 contains the following information for each n-th time step:

- Heading, giving the time step number and simulation time value.
- Nodal coordinates and values of the dependent variables.

4. File number 11. This file is written when a flow simulation is performed, IMODL = 1 or 2 (group 3, col. 1-5) and the plotting control parameter NPLOT is greater than zero. For NPLOT = n, the file contains the following information for each n-th time step:

- Heading, giving the time step number and time value.
- coordinates of the element centroids and Darcy velocity of each active phase.

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8 INPUT DATA PREPARATION

8.1 GENERAL CONSIDERATIONS

SAMFT1D is designed to perform the numerical solution of one problem or several consecutive problems in a single computer run. The code is intended to handle single-phase and multiphase fluid flow and solute transport problems. Three types of multiphase flow situations can be handled. These include: (1) three-phase flow of water (w), NAPL (n), and gas (a), (2) two-phase flow of water and NAPL in the three-phase w-n-a system, and (3) two-phase flow of NAPL and water. For single-phase flow, hysteresis can also be taken into account. Any set of consistent units may be used for both flow and transport simulations. However, the input of flux and concentration data must follow the procedure described in Section 8.2.

Several features are incorporated into SAMFT1D for automatic generation of a substantial portion of input required for the numerical analysis of a single-phase or multiphase problem. These are summarized below.

(1) Mesh generation option. This option is invoked by choosing the input variable IBCGR. If IBCGR=1, mesh-centered grids are generated for one active phase flow and single or multiple phase transport problems. If IBCGR=1, block-centered grids will be used for finite difference approximation to multiphase flow cases.

(2) Default initial value option. This option is used for initialization of primary dependent variables. For multiphase flow problems, it is invoked by setting IMODL=1, or 2, and IDFVAR=1, 2, 3, or 4. The code will automatically generate all the primary variables at all nodes according to capillary and gravity equilibrium conditions using water pressure, potential or saturation profiles from input data, as discussed in Section 3.3.1.3.

(3) Time step generation option. Time steps to be used in the numerical analysis of a transient flow problem is generated automatically. This option may be invoked by setting an input

control parameter ITSGN=1, and designed to use for flow simulation.

(4) Default values for element Darcy velocity and phase saturation. For a solute transport simulation, default values of Darcy velocity components and saturation are used to generate element velocities and phase saturation values. If desired, the generated data can be overridden by the correct data supplied to the code.

8.2 INPUT OF FLUX AND CONCENTRATION DATA

In the SAMFT1D code, input data pertaining to fluid and solute fluxes and concentration are handled differently for single-phase and multiphase simulations. The following convention must be adhered to in preparing input files for single-phase flow and transport problems:

(1) Nodal values of fluid fluxes must correspond to the volumetric water fluxes at the nodes.

(2) Nodal concentration values supplied to the code must be expressed in terms of dissolved contaminant mass per unit volume of water.

(3) Nodal values of solute fluxes must correspond to the dissolved mass fluxes of the contaminant in the water phase.

The following convention must be adhered to in preparing input files for multiphase flow and transport problems:

(1) Nodal values of fluid fluxes must correspond to the mass fluxes of fluid phases concerned in the flow simulation.

(2) Nodal concentration values supplied to the code must be expressed in terms of mass fraction defined as the mass of dissolved contaminant in the water phase per unit mass of water.

(3) Nodal values of solute fluxes must correspond to the total mass fluxes of the contaminant (as contributed from all fluid phases) at the nodes.

(4) For an injection well node, the total partitioned fluid flux at the node, Q_{TI}, must be determined from:

$$Q_{TI} = \rho_w Q_{wI} + \rho_n Q_{nI} \kappa_n + \rho_a Q_{aI} \kappa_a$$

where $\rho_w Q_{wI}$, $\rho_n Q_{nI}$, and $\rho_a Q_{aI}$ denote mass fluxes of water, NAPL and air, respectively, and κ_n and κ_a are the partitioning coefficients for the NAPL and air phase. Note that κ_n and κ_a relate concentrations in the NAPL and air to concentration in water, respectively. Either phase partitioning coefficient may be set to zero if the phase concerned is absent.

8.3 RESTART PROCEDURE

A restart option is provided in the code for continuation of the solution of a time-dependent problem. To use this option, the user must provide data pertaining to initial nodal values of the dependent variables. These nodal values are to be supplied as input data on a FORTRAN data file on unit 8. If the restart option is selected, the user should adopt the following procedure:

(1) Before restarting, a provision must be made in the preceding run for the code to write the last set of nodal values (computed at the final time step) on file unit 8. This is achieved by setting the value of the input variable NOWRIT to 1.

(2) Prepare input data for unit 5 of the restart run in the usual manner but keeping in mind that the initial conditions of the new problem can be derived from information contained in file unit 8. Note also that the variable NONU must be set to 2 and NOWRIT must be set to 0.

8.4 INPUT RECORDS

The main stream of input data is to be supplied from input file unit 5 (TAPE5). The code is capable of handling more than one problem in a single computer run. The types of problems considered by the program include: (1) saturated groundwater flow, (2) variably saturated water flow, (3) transport of a non-conservative (or conservative) species in variably saturated (or saturated) porous media, (4) multiphase flow of water, NAPL and air, and (5) transport of a non-conservative (or conservative) species in porous media saturated with multiphase fluids.

To facilitate data entry, the input data in unit 5 is divided into 22 groups, arranged as follows:

1. Problem control number
2. Problem title
3. Simulation control parameters
4. Time stepping, iteration control and gravitational parameters
5. Input and output control parameters
6. Temporal discretization data
7. Default initial condition for fluid flow problem
8. Initial condition for solute transport problem
9. Material properties for flow simulation
10. Soil-solute transport parameters
11. Grid generation parameters
12. Layered grid data
13. Boundary condition control record

14. Steady-state boundary condition data

15. Transient Dirichlet boundary condition data

16. Transient flux boundary condition data

17. Initial condition data

18. Transport simulation control data

19. Default velocity and phase saturation data

20. Observation node data

21. Observation node numbers

22. Output time specification data

The above sequence must be strictly followed when entering data into the program. Following are descriptions of the input variables and data formats.

*** The following data groups are required for each problem.

1. Problem control number (2I5)

One record.

Col.	1-5	IDPROB:	Problem identification number.
	6-10	IEXEC:	Parameter indicating if the code needs to be fully executed after setting up the problem, = 1 if yes, = 0 if no.

2. Problem title (A80)

One record.

Col. 1-80	TITLE:	Title of problem.

3. Simulation control parameters (15I5)

One record.

Col. 1-5	IMODL:	Parameter indicating the type of modeling required; = 0 for solute transport modeling, = 1 for single or multiphase flow modeling, = 2 simultaneous flow and transport modeling.
6-10	NTPHAS:	Total number of fluid phases that may exist in the flow system.
11-15	NMPHAS:	Number of active fluid phases. Note that NMPHAS ≤ NTPHAS. For a single-phase flow problem, set NMPHAS = 1.
16-20	IHYST:	Parameter indicating if hysteresis is to be included in the flow simulation; = 1 if yes, = 0 if no. For KPROP = 1 or NTPHAS = 1 the code automatically sets IHYST = 0. Note also that IHYST = 0 if only transport simulation is performed.
21-25	NVAR:	Total number of dependent variables for which nodal values are to be computed, = 1 if IMODL = 0, = NMPHAS if IMODL = 1, = NMPHAS + 1 if MODL = 2.
26-30	ISSTA:	Parameter indicating if the required analysis is a steady-state analysis for single phase flow and/or transport; = 1 if yes, = 0 if no. Note that for multiphase simulation ISSTA is to be set equal to 0.

31-35	ITSGN:	Parameter indicating if simulation time values are to be generated by the code; = 0 if no, and simulation time values are to be supplied to the code, = 1 if yes and computational time step values are to be determined by the code during the flow solution based on the rate of nonlinear convergence, = 2 if yes and time step values are to be supplied by the code (This option is not used for single-phase analysis). Note: The option of ITSGN = 1 is used for cases involving flow simulation (IMODL = 1) or combined flow/transport simulation (IMODL = 2). The remaining options of ITSGN = 0 and 2 are reserved for cases involving multi-phase transport simulation only.
36-40	NTS:	Number of time steps. Set NTS = 1 if a steady-state analysis is required.
41-45	NE:	Total number of elements or grid blocks.
46-50	NMAT:	Number of different porous soil materials.
51-55	KPROP:	Parameter indicating the form of relative permeability and capillary pressure data; = 0 for functional form, = 1 for tabulated form. KPROP must be set to 0 when dealing with single-phase flow problem.
56-60	NONU:	Parameter indicating if the initial condition differs from the default initial condition data described in record group 7 or 8; = 0 if no, = 1 if yes and initial condition data are to be input as part of this input file (see group 17),

= 2 if yes and initial condition data are to be read from a restart file on unit 8.

4. Time stepping,iteration control and gravitational parameters (3I5,6E10.3)

One record.

Col. 1-5	IKALL:	Parameter indicating the type of time stepping scheme for the solute transport simulation; = 1 for backward difference scheme, = 0 for central difference scheme. Note that IKALL is automatically set to 1 for a steady-state analysis. For the fluid flow simulation, the code automatically selects the backward difference scheme.
6-10	NITMAX:	Maximum number of nonlinear iterations allowed per time step of the flow simulation. Suggested values of NITMAX = 10 and 20 for transient and steady-state simulations, respectively.
11-15	ICONVG:	Convergence criterion option; = 1 for relative tolerance, = 2 for absolute tolerance.
16-25	HTOL:	Equivalent fresh-water head tolerance to be used in the nonlinear solution of the flow equation. Suggested value is $0.0 < \text{HTOL} \leq 0.01$ m.
26-35	STOL:	Phase saturation tolerance to be used in the nonlinear solution of the flow equation. Suggested value is $0.0 < \text{STOL} \leq 0.005$.
36-45	GCONST:	Gravitational acceleration constant.
46-55	PATM:	Atmospheric pressure (absolute).

56-65	RPTOL:	Relative pressure tolerance to be used in the nonlinear solution of the flow equation for multiphase flow analysis.
66-75	RSTOL:	Relative saturation tolerance to be used in the nonlinear solution of the flow equation for multiphase flow analysis.

5. Input and output control parameters (14I5)

One record.

Col. 1-5	NVREAD:	Parameter specifying if element velocity and saturation data for each fluid phase are to be input; = 0 if no velocity input is needed (this option is used for a flow run or for transport in uniform flow), = 1 if the velocity data is to be input using a separate data file unit number 9. Note the NVREAD is set to 0 if IMODL = 1 OR 2.
6-10	IOUTLT:	Not used and leave blank.
11-15	NPIN:	Number of nodes for which initial nodal values of the dependent variables are to be input as part of this input file. NPIN is automatically set to 0 unless NONU = 1.
16-20	IPRD:	Parameter indicating if printout of mesh and initial condition data is to be deleted; = 0 if no, = 1 if yes.
21-25	NVWRIT:	Parameter specifying if the computed values of element velocities and saturation for each fluid phase are to be written on file unit 9; = 0 if no, = 1 if yes and output is to be written for each time step,

= 2 if yes and output is to be written for selected time steps as specified in record group 22.
Note: set NVWRIT to 0 if IMODL = 0, or IMODL = 2.

26-30	NVPR:	Parameter controlling the printout of computed element velocities; = 0 if no output is to be written, = n if the output is to be written for each n-th time step.
31-35	NPLOT:	Parameter indicating if time and computed nodal values of the dependent variables are to be written on file unit 10 for use in subsequent plotting; = 0 if no output is to be written, = n if the output is to be written for each n-th time step. For flow simulation (IMODL = 1 or 2) values of velocity components at element centroids are also written on file unit 11.
36-40	NSTEP:	Parameter controlling the printout for computed nodal values of dependent variables; = 0 if no output is to be written, = n if the output is to be written for each n-th time step.
41-45	IOBSND:	Parameter indicating if the values of dependent variables at some specified nodes are to be recorded for all the time steps (see groups 20 and 21); = 1 if yes, = 0 if no.
46-50	IMBAL:	Parameter specifying if mass balance calculation is required, = 1 if yes, = 0 if no.
51-55	NOWRIT:	Parameter indicating if the computed nodal values of the dependent variables at

		the final time level are to be written on file unit 8; = 1 if yes, = 0 if no.
56-60	IPRCHK:	Computation print check parameter (used for debugging purposes); = 0 if print check is not needed, ≥ 1 if print check is needed. For multiphase flow simulation, a three-level print check option is used; = 1 if print check of time stepping, iteration and boundary flux information is needed, = 2 if in addition printout of Jacobian matrix is needed, = 3 if a detailed printout is needed.
61-65	NPRCON:	Parameter indicating if computer nodal values of the dependent variables are to be printed at specified time values indicated in record group 22(a); = 0 if no, = n if yes and output is to be written at n specified time values.
66-70	IPWOUT:	Parameter indicating the output requirement for single-phase flow analysis; = 1 if pressure head values are to be printed, = 0 if pressure values at the nodes are to be printed. For multiphase flow analysis, IPWOUT is automatically set by the code as 1.

Note: If NPRCON = 0, output will be written at specified time step intervals as controlled by the parameters NVPR, NPLOT and NSTEP. If NPRCON ≠ 0, the output will also be written for the user-selected actual time values (see group 22).

6. Temporal discretization data

*** Omit this group if a steady-state analysis is required, ISSTA = 1 (group 3, col. 21-25).

(a) Time values (8E10.3)

*** Omit unless ITSGN = 0 (group 3, col. 26-30)

Number of records = NTS/8 + 0 or 1.

Col. 1-10	TMVEC(I):	Time values at the end of time steps 1
11-20	I=1,	through NTS.
etc.	NTS	

(b) Time discretization parameters (4E10.3)

*** Omit unless ITSGN = 1 (group 3, col. 26-30)

One record.

Col. 1-10	TIMA:	Starting time value of the simulation.
11-20	TIN:	Value of the first time step.
21-30	TMIN:	Minimum allowable time step size.
31-40	TMAX:	Maximum allowable time step size.
41-50	TEND:	Final time value of the simulation.

(c) Time discretization parameters (3E10.3,I5)

*** Omit unless ITSGN = 2 (group 3, col. 26-30)

Number of records = as many as needed.

Each record contains the following information:

Col. 1-10	TMST:	Starting time value.
11-20	TMEND:	Ending time value.
21-30	DTS:	Time step used between TMST and TMEND.
31-35	IPAUSE:	Parameter indicating if this is the last record for subgroup 6c; = 1 if yes, = 0 if no.

7. Default initial condition data

(a) Initial Condition for fluid flow problem

*** Omit if IMODL = 0 (group 3, col. 1-5).

The code provides three options for the specification of default initial condition for the simulation of fluid flow problems by specifying initial water pressure, potential or saturation profiles, as illustrated in Figure 8.1. In each option it is assumed that the initial saturation of the second fluid phase and the initial pressure of the third fluid phase are constant (atmospheric).

(i) First record (2I5,3E10.3)

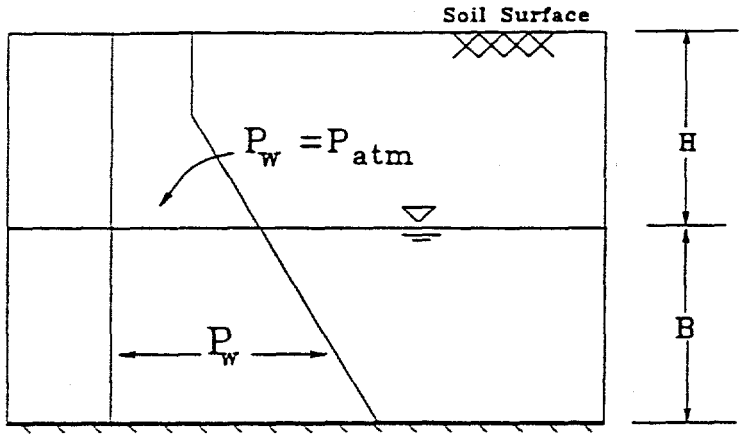
One record. Col. 11-20 may be left blank or set to zero if dealing with a single phase flow problem.

Col. 1-5 IDFVAR: Initial condition identifier;
= 1 if vertical profile of the initial pressure (p_w) of the first fluid phase (wetting phase) is to be specified (see Table 8.1 for the convention used in numbering fluid phases);
= 2 if vertical profile of the initial potential of the wetting phase (Φ_w) is to be specified;
= 3 if vertical profile of the initial saturation of the wetting phase (S_w) is to be specified;
= 4 if dealing with horizontal flow problem for which initial value of water pressure is specified.

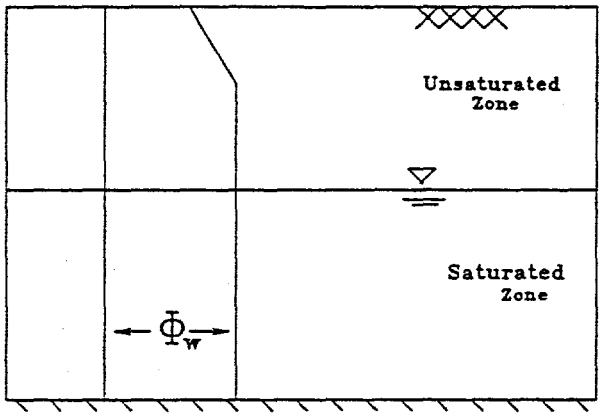
6-10 NCPONT: Number of control points required to specify the distribution of the initial function corresponding to the specified value of IDFVAR.

11-20 HIDFAL(1): Default value of initial saturation of the second active fluid phase.

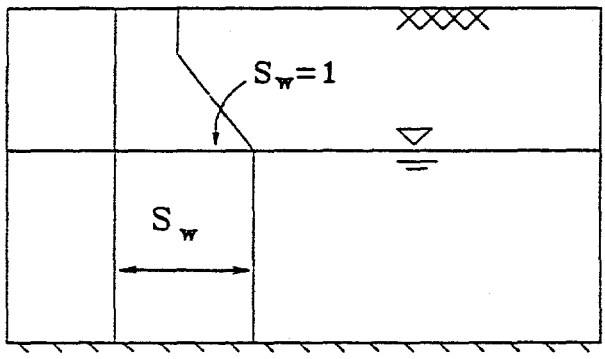
21-30 HIDFAL(2): Default value initial (atmospheric) pressure of the third active fluid phase.



(a) Prescribed initial P_w (IDFVAR =1)



(b) Prescribed initial Φ_w (IDFVAR =2)



(c) Prescribed initial S_w (IDFVAR =3)

Figure 8.1 Three default initial condition options offered by the code for multiphase flow modeling.

31-40 HIDFAL(3): Depth from the top of the flow domain to the water table. Leave blank if the grid is horizontal.

(b) Initial function data (2I5,2E10.3)

*** Omit if NCPONT = 0.

Col. 1-5 N: Control point number (see Figure 8.2)

6-10 ISOIL(N): Soil type identification number.

11-20 ZP(N): Value of coordinate along which distribution of initial function is described; vertical coordinate value if IDFVAR $\leq$ 3, or horizontal coordinate value if IDFVAR = 4.

21-30 FZP(N: Value at the control point on the profile of the initial function corresponding to the specified value of IDFVAR.
Note: Control points (N = 1 to NCPONT) must be numbered sequentially starting from the minimum to maximum coordinate values of the flow domain.

8. Initial condition for solute transport problem (E10.3)

*** Omit if IMODL = 1 (group 3, col. 1-5).

One record

Col. 1-10 CIDFAL: Default initial value of solute concentration.

9-I. Material properties for flow simulation

*** Omit this group if IMODL = 0 (group 3, col. 1-5).

(a) Soil properties (3E10.3)

Number of records = NMAT (group 3, col. 46-50)

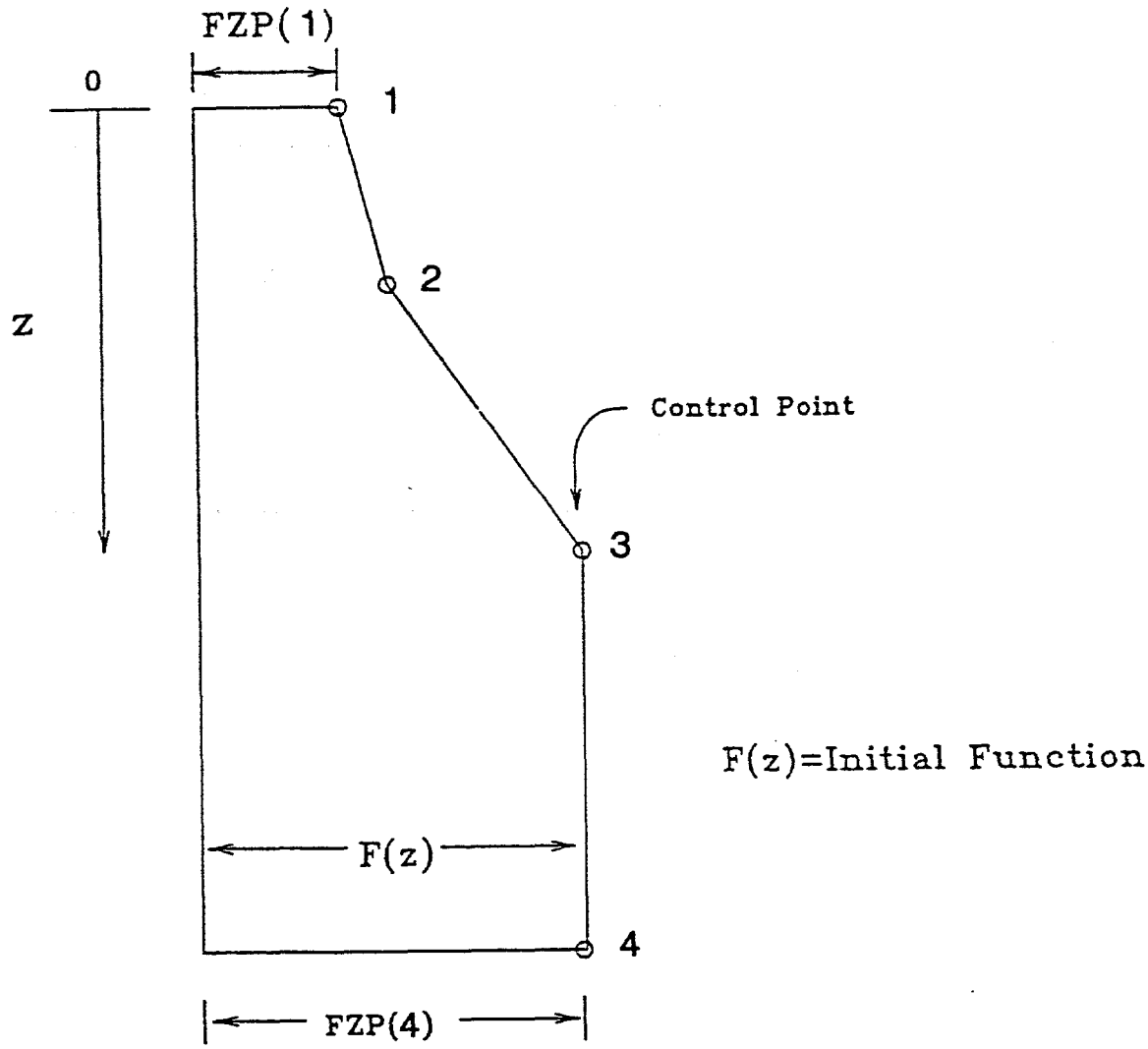


Figure 8.2 Representation of an initial condition function.

Table 8.1. Fluid phase numbering convention used by the code.

Fluid System Considered	Fluid phase numbering		
	Phase 1	Phase 2	Phase 3
water, NAPL, air (or vapor)	water	NAPL	air (or vapor)
water, NAPL	water	NAPL	--
water, air	water	air	--
water	water	--	--

Col.	1-10	PROP(I,1):	Vertical component of intrinsic permeability of material I.
	11-20	PROP(I,2);	Volume compressibility of material I.
	21-30	PROP(I,3):	Effective porosity of material I at reference pressure.
	31-40	SNIRWN(I):	Irreducible NAPL saturation for the water-NAPL (w-n) fluid system.
	41-50	SNSTR(I):	Threshold (critical) NAPL saturation beyond which air-water interface ceases to exist. Default value of SNSTR(I) is the value of SNIRWN(I).
		Note:	For single phase flow simulation, leave col. 31-50 blank.

(b) Fluid Properties (3E10.3)

Number of records = NMPHAS (group 3, col. 6-10). The numbering of fluid phases is described in Table 8.1 for the various situations considered by the code.

Col.	1-10	FPROP(I,1):	Reference density of fluid phase I.
	11-20	FPROP(I,2):	Reference dynamic viscosity of fluid phase I.
	21-30	FPROP(I,3):	Compressibility of fluid phase I (see definition on Pages 2-15 - 2-16).

(c) Relative Permeability and Capillary Functional Parameters for water-air (w-a) fluid system

*** Omit if KPROP = 1 (group 3, col. 51-55) or NTPHAS = 1 (group 3, col. 6-10).

Number of records = NMAT. Typically record I contains parameters for soil material I.

Col.	1-10	PROP(I,7):	Residual water saturation (S_{wr}).
	11-20	PROP(I,8):	Exponent (N) of the Brooks-Corey relative permeability versus phase saturation function. Set PROP(I,8) = 0

if the van Genuchten k_{rw} function is to be used instead of the Brooks-Corey function. For single-phase flow problem, the Brooks-Corey k_{rw} function is expressed as $k_{rw} = (\bar{S}_w)^N$ where $\bar{S}_w$ is the effective water-phase saturation. For multiphase flow problem, k_{rw} is expressed as $k_{rw} = (\bar{S}_w)^{N+2}$.

21-30 PROP(I,9): Leading coefficient (α) of the van Genuchten function:

$$\bar{S}_w = [1 + (\alpha|\psi|^{\beta})]^{-\gamma}$$
where $\psi = (p_w - p_a)/\rho_w g$.

31-40 PROP(I,10): Power index (β) of the van Genuchten function.

41-50 PROP(I,11): Power index (γ) of the van Genuchten function. If PROP(I,11) is left blank, the code will assume that $\gamma = 1\text{-}1/\beta$.

51-60 PROP(I,12): Interfacial surface tension (σ_{aw}) between fluid phases a and w.

61-70 PROP(I,13): Interfacial surface tension (σ_{nw}) between fluid phases n and w.

71-80 PROP(I,14): Interfacial surface tension (σ_{an}) between fluid phases a and n.

Note: (1) If performing single-phase flow simulation, col. 61-80 should be left blank.

(2) For a case involving hysteresis (IHYST = 1, group 3, col. 16-20), the function parameters correspond to the main drainage (drying) curve of the hysteretic capillary pressure versus saturation relations.

(d) Tabulated Relative Permeability and Capillary Pressure Data

*** Omit if KPROP = 0 (group 3, col. 56-60) or NTPHAS = 1 (group 3, col. 6-10).

Number of record sets = NMAT (group 3, col. 51-55). Typically, record set I contains the following data for soil material I:

(i) Control Record (2I5,3E10.3)

One record.

Col. 1-5	NRPH12(I):	Number of row entries required to define the constitutive relationships for fluid phase 1 versus 2. See Table 8.1 for fluid phase numbering convention.
6-10	NRPH23(I):	Number of row entries required to define the constitutive relationships for fluid phase 2 versus 3 and phase 3 versus 1. Set NRPH23(I) = 0 if dealing with a two-phase flow system.
11-20	PROP(I,7):	Irreducible water-phase saturation (S_{wr}).
21-30	PCNSW1(I):	Capillary pressure between water and NAPP at $S_w = 1$ in the water-NAPL (w-n) system.
31-40	AKSTAR(I):	Relative permeability of NAPL at the residual saturation of water in the water-NAPL (w-n) fluid system.

(ii) Constitutive relationships for phase 1 versus 2 (4E10.3)

Number of records = NRPH12(I). Typical record for entry J is as follows:

Col. 1-10	SPH1(J,I):	Saturation of phase 1 (the wetting aqueous phase). Values of SPH1(J,I) must be arranged in ascending order with the maximum value equal to 1.
11-20	RKPH1(J,I):	Relative permeability of phase 1.
21-30	RKPH21(J,I):	Relative permeability of phase 2 with respect to phase 1.
31-40	PCPH21(J,I):	Capillary pressure between phases 2 and 1. Leave blank if capillary pressure effects are to be neglected.

(iii) Constitutive relationships for phase 2 versus phase 3 (5E10.3)

*** Omit if NRPH23(I) = 0.

Number of records = NRPH23(I). Typical record for entry J is as follows:

Col. 1-10	SPH3(J,I):	Saturation of phase 3. Values of SPH3(I,J) must be arranged in ascending order.
11-20	RKPH3(J,I):	Relative permeability of phase 3.
21-30	RKPH23(J,I):	Relative permeability of phase 2 with respect to phase 3.
31-40	PCPH32(J,I):	Capillary pressure between phases 3 and 2. Leave blank if capillary effects are to be neglected.
41-50	PCPH31(J,I):	Capillary pressure between phases 3 and 1. Leave blank if capillary effects are to be neglected.

9-II. Additional Data for Hysteretic Flow Simulation

*** Omit this group if IHYST = 0 (group 3, col. 16-20).

(a) Parameters for Main Imbibition Curve (4E10.3)

Number of records = NMAT.

Col. 1-10	PROP(I,15):	Maximum water-phase saturation (S_{ws}) of soil material number I. Default value of $S_{ws} = 1$.
11-20	PROP(I,16):	Leading coefficient (α^w) of the van Genuchten function of water saturation versus capillary head.

(b) Initial Hysteresis Index and Phase Saturation (I5,E10.3,4I5)

Number of records = as many as needed.

Col.	1-10	KHYSTV:	Initial value of hysteresis index for the wetting phase (w); = -1 if initially draining, = 1 if initially imbibing.
	6-15	SWINTV:	Initial value of the wetting-phase saturation; Leave blank or set to 0.0 if IDFVAR = 3 (see group 7, col. 1-5).
	16-20	IELST:	Starting element number.
	21-25	IELEND:	Ending element number.
	26-30	IELINC:	Element number increment.
	31-35	IPAUSE:	Parameter indicating if this is the last record in the group; = 1 if yes, = 0 if no.

10. Soil-solute transport parameters

*** Omit if group if IMODL = 1 (group 3, col. 1-5).

(a) Soil physical transport parameters (5E10.3)

Number of records = NMAT (group 3, col. 46-50)

Col.	1-10	PROPJ(I,1):	Longitudinal dispersivity, α_L, of soil material I.
	11-20	PROPJ(I,2):	Tortuosity factor, τ, of material I.
	21-30	PROPJ(I,3):	Exponent n of the equation: $D_\ell^* = (\phi\tau S_\ell^n) D_{m\ell}$ is used to compute the apparent molecular diffusion of solute in fluid phase ℓ. If the Millington-Quirk diffusion coefficient expression is to be used, then set n=10/3, and $\tau = \phi^{1/3}$.
	31-40	PROPJ(I,4):	Effective porosity, ϕ, of soil material I.
	41-50	PROPJ(I,5):	Bulk density, ρ_b, of soil material I.

(b) Molecular diffusion coefficients (3E10.3)

One record.

Col. 1-10	DMPHAS(I):	Molecular diffusion, D_{mI}, of solute in
11-20	I=1,	fluid phase I. See Table 8.1 for fluid
etc.	NTPHAS	phase numbering convention.

(c) Soil-solute transport parameters (2E10.3)

Number of records = NMAT (group 3, col. 36-40).

Col. 1-10	RPROP(I,1):	Solute decay coefficient, λ, of material I. For a conservative solute species set RPROP(I,1) = 0.0. Note: $\lambda = \ln 2/t_{1/2}$, where $t_{1/2}$ = half life.
11-20	RPROP(I,2):	Distribution coefficient (solute partitioning coefficient between fluid phase 1 and soil material I), k_d. Note: the units for k_d must be the reciprocal of the units for bulk density. For a non-adsorbed solute species set RPROP(I,2).

(d) Fluid Densities (3E10.3)

*** Omit if NMPHAS = 1 (group 3, col. 11-15) or IMODL = 2 (group 3, col. 1-5).

One record.

Col. 1-10	FPROP(I,1):	Density of fluid phase I.
11-20	I=1,	
etc.	NTPHAS	

(e) Fluid-pair partitioning coefficients and solubility limit (3E10.3)

*** Omit if NMPHAS = 1 (group 3, col. 11-15).

One record.

Col. 1-10	PCOEF(1):	Solute partitioning coefficient between fluid phases 1 and 2.

11-20	PCOEF(2):	Solute partitioning coefficient between fluid phases 1 and 3.
21-30	PCOEF(3):	Water-phase solubility limit (maximum dissolved concentration of the contaminant component in water. If PCOEF(I) is left blank, the code will assume unlimited solubility.

11. Grid generation parameters (2I5,F10.3,I5)

One record.

Col. 1-5	NLAYER:	Number of soil layers or zones that need to be discretized. These zones are numbered sequentially from top to bottom of the domain.
6-10	IBCGR:	Parameter indicating if a block-centered finite difference or a mesh-centered finite element grid is to be used, = 0 for a mesh-centered grid (used for cases involving one active fluid phase, NMPHAS = 1 or multi-phase transport simulation only). = 1 for a block-centered grid (used for multiphase flow simulation).
11-20	ACROS:	Cross-sectional area of the flow domain. Default value of ACROS = 1. For single-phase flow and transport simulations, ACROS is assumed by the code to be 1.
21-25	IHORGR:	Parameter indicating if the grid is oriented in a horizontal or vertical plane; = 0 if vertical plane, = 1 if horizontal plane.

12. Layered grid data (3I5,F10.3)

Number of records = NLAYER.

Col. 1-5	ILAYR:	Layer number.

6-10	NELM(ILAYR):	Number of elements (or grid blocks) in layer ILAYR.
11-15	IMATL(ILAYR):	Material number of layer ILAYR.
16-25	THL(ILAYR):	Thickness of layer ILAYR.

Note: Each layer is divided into a number of equal-length grid blocks (or elements). The sum of NELM(ILAYR) for all layers must be equal to NE specified in group 3, col. 41-45.

13. Boundary condition control record (4I5)

In supplying boundary condition data to the code, it is necessary to correctly assign sequential number(s) of the dependent variable(s) being considered in the simulation run. This ordering notation for the dependent variables, shown in Table 8.2, can be easily adapted to a general case of dual flow and transport simulation and simpler cases involving flow or transport simulation only. It should also be noted that prescribed flux and concentration data must be input following the procedure described in Section 8.2.

One record.

Col. 1-5	NBTO:	Number of steady-state Dirichlet boundary conditions.
6-10	NDFLUX:	Number of steady-state prescribed flux boundary conditions.
11-15	NBHVAR:	Number of transient Dirichlet boundary conditions.
16-20	NBFVAR:	Number of transient flux boundary conditions.
21-25	NBCND1:	Identification number of top boundary condition for multiphase flow at node 1; = 1 for one or more fluid injection fluxes specified, = 2 for one or all active phase injection pressures specified, = 3 for water and/or NAPL injection fluxes specified, and air pressure equal to atmospheric pressure.

26-30	NBCNDN:	Identification number of bottom boundary condition for multiphase flow at the last node; = 1 if total liquid production flux is specified, = 2 if one boundary pressure specified. Note: for transport or single-phase flow simulation, leave col. 21-30 blank.

For a multiphase vertical flow problem, the surface boundary at node 1 should be treated as an influx boundary with either injection pressure or flux specified. The boundary conditions at the last node is regarded as efflux conditions. The total liquid flux should be provided for the last node if production or sink flux conditions are needed. At the bottom boundary, only one pressure needs to be specified when Dirichlet boundary conditions apply.

14. Steady-state boundary condition data (2I5,E10.3)

(a) Steady-state Dirichlet boundary conditions (2I5,E10.3)

*** Omit if NBTO = 0 (group 13, col. 1-5).

Number of records = NBTO.

Col.	1-5	NODV(I):	Node number concerned with a Dirichlet boundary condition.
	6-10	MDEGB(I):	For the fluid flow problem, MDEGB(I) corresponds to the identification number of the fluid phase for which the injection pressure is prescribed (see Table 8.1) and set MDEGB(I) = 0 for outflow pressure boundary condition which will be applied to all fluid phases. For the solute transport problem, MDEGB(I) corresponds to the governing equation number of the transport equation (see Table 8.2).
	11-20	VALVO(I):	Prescribed value of the concerned variable (fluid phase pressure or solute concentration) at the specified node.

Table 8.2. Dependent-variable numbering convention used by the code, p_ℓ and q_ℓ denote pressure and volumetric flux of fluid phase ℓ, respectively, and q_c denotes solute mass flux.

Problem Type / Description	Governing equation number and corresponding pair of primary dependent variable and associate material flux			
	1(w) or 1(c)	2(n or a) or 2(c)	3(a) or 3(c)	4(c)
Flow of a three-phase fluid (w,n,a) system	(p_w,q_w)	(p_n,q_n)	(p_a,q_a)	-
Flow of a two-phase fluid (w,n) or (w,a) system	(p_w,q_w)	(p_n,q_n) or (p_a,q_a)	-	-
Flow of a single-phase fluid (w) system	(p_w,q_w)	-	-	-
Single-component solute transport	(c,q_c)	-	-	-
Dual simulation of flow and transport in a three-phase fluid system	(p_w,q_w)	(p_n,q_n)	(p_a,q_a)	(c,q_c)
Dual simulation of flow and transport in a two-phase fluid system	(p_w,q_w)	(p_n,q_n) or (p_a,q_a)	(c,q_c)	-
Dual single-phase flow and transport simulation	(p_w,q_w)	(c,q_c)	-	-

(ℓ) = governing flow equation for fluid phase ℓ (where ℓ = w, n or a), and
(c) = governing transport equation for solute component.

(b) Steady-state flux boundary condition data (2I5,2E10.3)

*** Omit if NDFLUX = 0 (group 13, col. 6-10).

Number of records = NDFLUX. Note that the outward flux is taken to be negative and the inward flux is taken to be positive.

Col.	1-5	NODF(I):	Node number concerned with a constant flux boundary condition of a particular governing flow or transport equation.
	6-10	MDEGF(I):	For the fluid flow problem, MDEGF(I) corresponds to the identification number of fluid phase for which the flux is prescribed. In a case of an outflow boundary node or a sink node, set MDEGF(I) = 0. For the solute transport problem, MDEGF(I) corresponds to the governing equation number of the transport equation.
	11-20	FLUXVO(I):	For the fluid flow problem, FLUXVO(I) denotes fluid volumetric flux at the specified node. This flux corresponds to the total flux of liquids if MDEGF(I) = 0. Otherwise, it corresponds to the flux of the specified fluid phase. For the transport equation, FLUXVO(I) corresponds to the solute mass flux prescribed at the node.
	21-30	QVALV(I):	For the fluid flow equation, QVALV(I) is to be left blank. For the transport equation, QVALV(I) corresponds to the total fluid flux at the specified node. For a single phase simulation, this flux corresponds to water volumetric flux, Q_{WI}. For a multiphase simulation, the flux corresponds to the total partitioned fluid mass flux, Q_{TI}, defined below.

Note: (1) The sign convention for fluid and solute mass fluxes is positive for influxes and negative for effluxes. In performing solute transport simulation, the code automatically treats the efflux boundary node. Hence such a node can be excluded from group 14b.

(2) The total partitioned fluid mass flux at node I (Q_{TI}) is defined as
$Q_{TI} = \rho_w Q_{wI} + \rho_n Q_{nI} \kappa_n + \rho_a Q_{aI} \kappa_a$
where $\rho_w Q_{wI}$, $\rho_n Q_{nI}$, and $\rho_a Q_{aI}$ denote mass fluxes of water, NAPL and air, respectively, and κ_n and κ_a are the partitioning coefficients for the NAPL and the air phase.

15. Transient Dirichlet boundary condition data

*** Omit if NBHVAR = 0 (group 13, col. 11-15).

Number of record sets = NBHVAR.

Each set contains the following records:

(a) Control record (4I5)

One record.

Col. 1-5	NDHVAR(I):	Node number concerned with a time-dependent Dirichlet boundary condition.
6-10	MDEGBT(I):	For the fluid flow problem, MDEGBT(I) corresponds to the identification number of the fluid phase for which the injection pressure is prescribed, and set MDEGBI(I) = 0 for outflow presure boundary condition which will be applied to all active phases. For the solute transport problem, MDEGBT(I) corresponds to the governing equation number of the transport equation.
11-15	NTSNDH(I):	Number of control points on the time graph of the boundary condition at the node.
16-20	ITVARH(I):	Parameter indicating the time variation of the prescribed function data; = 0 for continuous variation, = 1 for discontinuous (stepped) variation.

(b) Time value records (8E10.3)

Number of records = NTSNDH(I)/8 + 0 or 1 (group 15a, col. 11-15).

Col.	1-10	TMHV(I,J):	Sequential time values corresponding to
	11-20	J=1,	the control points on the time graph
	etc.	NTSNDH(I)	depicting temporal variation of the prescribed dependent variable (fluid phase pressure or solute concentration).

(c) Functional value records (8E10.3)

Number of records = NTSNDH(I)/8 + 0 or 1 (group 15a, col. 11-15).

Col.	1-10	HVTM(I,J):	Prescribed values of the concerned
	11-20	J=1,	variable (fluid phase pressure or solute
	etc.	NTSNDH(I)	concentration at the corresponding time values, TMHV(I,J).

16. Transient flux boundary condition data

*** Omit if NBFVAR = 0 (group 13, col. 16-20).

Number of record sets = NBFVAR.

Each set contains the following records:

(a) Control records (4I5)

One record.

Col.	1-5	NDFVAR(I):	Node number concerned with a time-dependent flux boundary condition.
	6-10	MDEGFT(I):	For the fluid flow problem, MDEGFT(I) corresponds to the identification number of fluid phase for which the flux is prescribed. In a case of an outflow boundary or a sink node, set MDEGFT(I) = 0. For the solute transport problem, MDEGFT(I) corresponds to the governing equation number of the transport equation.
	11-15	NTSNDF(I):	Number of control points on the time graph of the flux boundary condition at the node.
	16-20	ITVARF(I):	Parameter indicating the time variation of the prescribed nodal flux data;

= 0 for continuous variation,
= 1 for stepped variation.

(b) Time value records (8E10.3)

Number of records = NTSNDF(I)/8 + 0 or (group 16a, col. 11-15).

Col.	1-10	TMHF(I,J):	Sequential time values corresponding to the control points on the graph depicting temporal variation of the flux boundary condition at the node.
	11-20	J=1,	
	etc.	NTSNDF(I)	

(c) Flux value cards (8E10.3)

Number of records = NTSNDF(I)/8 + 0 or 1 (group 16a, col. 11-15).

Col.	1-10	FVTM(I,J):	For the fluid flow problem, FVTM(I,J) denotes fluid flux at the specified fluid phase. For the transport equation, FVTM(I,J) corresponds to the solute mass flux at the node.
	11-20	J=1,	
	etc.	NTSNDF(I)	

(d) Fluid flux value records (8E10.3)

*** Omit if IMODL = 1 (group 3, col. 1-5). Also omit if IMODL = 2 and MDEGFT(I) is less than NVAR (Group 3, Col. 21-25).

Number of records = NTSNDF(I)/8 + 0 or 1 (group 16a, col. 11-15).

Col.	1-10	QVTM(I,J):	Total fluid flux values corresponding to TMHF(I,J).
	11-20	J=1,	
	etc.	TNSNDF(I)	

17. Initial condition data

*** Omit if NONU = 0 or 2 (group 3, col. 56-60). Also omit if NPIN = 0 (group 5, col. 11-15).

Supply the initial condition data to the code according to one of the following formats:

(a) Format type 1 (I5,5F10.5)

To be used only when NPIN (group 5, col. 11-15) is less than NP.

(Note: NP = total number of nodes, and NPIN = number of nodes for which initial nodal values are to be read).

Number of records to be supplied = NPIN (group 5, col. 11-15).

Col. 1-5	N:	Node number.
6-15	HINT(N,J):	Initial value of primary dependent
16-20	J=1,NVAR	variable numter 1 through NVAR (group
etc.		3, col. 21-25). Table 8.3 provides the ordering of the primary variables for various simulations.
		Note that for multiphase flow problems, pressure and saturation values at node N corresponds to element values.
	CMP(N):	Initial mass of the modeled species component considered to be in the precipitated phase per unit volume of porous medium at node N.
		Note that CMP(N) is usually zero unless the initial concentration HINT(N,NVAR) corresponds to the water-phase solubility limit.

(b) Format type 2 (5E14.4)

To be used only for a restart run where initial values to be read correspond to the final set of nodal values obtained from a previous run. This set of nodal values can be obtained from file unit 8.

Number of records = NP

Col. 1-10	HINT(N,J):	Initial value of primary dependent variable
11-20	J=1,NVAR	number 1 through NVAR (group 3, col.
etc.		21-25). Table 8.3 provides the ordering of the primary variables for various simulations.
	CMP(N):	Initial mass of the modeled species component considered to be in the precipitated phase per unit volume of porous medium at node N.

Table 8.3. Primary dependent variables used by the code for various types of simulation.

Type of Simulation	Primary variable numbering 1	2	3	4
Three-phase flow of water, NAPL and air (w,n,a)	P_n	S_w	S_n	(c)
Two-phase (w,n, flow in (w,n,a) fluid system	P_n	S_n (NAPL) saturation	(c)	
Two-phase (w,n) flow in (w,n) fluid system	P_n	S_n (NAPL) saturation	(c)	
Single-phase water flow in (w,a) fluid system	P_w	(c)		
Single-component solute transport	c			

Note that for each combined flow/transport simulation, the concentration variable (c) is the additional variable following the flow variables.

18. Transport simulation control data (I5,3F10.3)

*** Omit if IMODL = 1 (group 3, col. 1-5). One record.

Col. 1-5	IVSTED:	Parameter indicating if the velocity field is steady state; = 1 if yes, = 0 if no.
6-15	WFAC:	Default value of transport upstream weighting factor. Leave blank if upstream weighting is not required.

19. Default velocity and phase saturation data (I5,4E10.3)

*** Omit if IMODL = 1 (group 3, col. 1-5).

Number of records = NMPHAS (group 3, col. 11-15).

Col. 1-5	IPHAS:	Fluid phase number.
6-15	SDFPH(IPHAS):	Default value of saturation of fluid IPHAS.
16-25	VXDFPH(IPHAS):	Default value of the Darcy velocity of fluid IPHAS.

20. Observation node data (I5)

*** Omit if IOBSND = 0 (group 5, col. 41-45).

One record.

Col. 1-5	NNOBS:	Number of nodes for which time history of computed values of dependent variable(s) is to be recorded.

21. Observation node numbers (16I5)

Number of records = NNOBS/16 + 0 or 1.

Col. 1-5 6-10 etc.	NDOBS(I): I=1, NNOBS	Node numbers of observation nodes.

22. Output time specification data

(a) Dependent variable output time values (8E10.3)

*** Omit if NPRCON = 0 (group 5, col. 61-65)

Number of records = NPRCON/8 + 0 or 1.

Col.			
	1-10	TMPRC(I),	Time values at which dependent variable
	11-20	I=1,	values should be written to the output
	71-80	NPRCON	file(s).

(b) Velocity output time values (2E10.3,2I5)

*** Omit unless NVWRIT = 2 (group 5, col. 21-25).

Number of records = as many as needed.

Each record contains the following information:

Col.			
	1-10	TSTVOP:	Starting time value for writing the velocity output on unit 9 for use in subsequent transport simulation. For the first record, TSTVOP must be set equal to TIMA (group 6b, col. 1-10).
	11-20	DTVOP:	Time increment for velocity output.
	21-25	NDTVOP:	Number of increments with constant value of DTVOP.
	26-30	IPAUSE:	Parameter indicating if this is the last record in group 20b; = 1 if yes, = 0 if no.

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9 OUTPUT

9.1 GENERAL CONSIDERATIONS

Line printer output from SAMFT1D is organized for each problem into categories of information. These categories are summarized as follows:

- Listing of general control input data supplied to the code by the user
- Listing of the generated mesh data
- Listing of boundary condition data
- Listing of initial condition data
- Listing of user-supplied steady-state values of element velocities and saturation
- Listing of user-supplied data pertaining to the nonzero flux nodes and flux values
- Listing of time stepping and nonlinear iterations for multiphase flow simulations
- Listing of inflow and outflow rates through boundaries for multiphase flow simulations
- Listing of element numbers and centroidal coordinates
- Listing of the input data supplied from file unit 9 for each time step
- Listing of information pertaining to the computation of element matrices and incorporation of boundary conditions performed by the code
- Listing of node numbers and values of pressure and saturation or concentration computed by the code. This listing is given for every n-th time step, where n is the value of NSTEP
- Listing of element numbers and phase saturation values for the elements that

contain more than one phase. This listing is given for every n-th time step, where n is the value of NSTEP

- Listing of element numbers and the components of Darcy velocity of each phase. This listing is given for every n-th time step, where n is the value of NVPR
- Listing of a mass balance budget if the mass balance option is selected.

9.2 OUTPUT CONTROL

Output streams are controlled by several control parameters, the values of which must be supplied to the code. Table 9.1 provides a summary of the procedures used to control various categories of output. The user should decide how much printed output is really needed for the problem simulated. For example, the mesh data and the boundary conditions are normally not needed in the restart run of the same problem.

Table 9.1 Output Control Parameters for File Number 6.

CONTROL PARAMETER	VALUE	MEANING
IPRD	0	List the printout of the entire mesh data as well as the initial condition.
IPRD	1	Suppress the printout of the entire mesh data as well as the initial condition.
NSTEP	n	For each n-th time step, print computed values of head or concentration (as the case may be), and print computed values of element water saturation (if variably-saturated flow analysis is performed). Note: When the value of NSTEP is greater than NTS (the total number of time steps of the simulation), the mentioned printout will be suppressed.
NVPR	n	For each n-th time step, print element numbers and computed values of Darcy velocity components at the element centroids. Note: When the value of NVPR is greater than NTS, the mentioned printout will be suppressed.
NPRCON	n	For n > 0, there are n specified time values at which the dependent variable values should be written on the output file.

NOTE: Values of IPRD, NSTEP, NVPR, and NPRCON are read from file number 5, described in Section 8.3. IPRD is the variable in group 5, cols. 16-20. NVPR, NSTEP and NPRCON are the variables in group 5, cols. 26-30, cols. 36-40, and cols. 61-65, respectively.

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10 INPUT AND OUTPUT FOR SAMPLE PROBLEMS

10.1 GENERAL CONSIDERATIONS

To demonstrate the utility of the code and familiarize the user with the input and output formats of the code, input data and computer output from five sample problems are provided. These are the one-dimensional single-phase and multiphase flow and transport problems.

The first problem (Section 10.2) was used to show the code capability and options for simulating single-phase unsaturated flow including effects of hysteresis on capillary pressure. These options are: (1) automatic mesh generation, (2) default initial saturation values, (3) entry of additional hysteresis parameters, (4) specification of time dependent pressure-prescribed boundary conditions, (5) computation and printout of Darcy velocity components and water saturations, (6) mass balance computation, and (7) printout control options.

The second problem (Section 10.3) was chosen to demonstrate the code options related to single-phase nonhysteretic flow modeling. These options are: (1) automatic mesh generation, (2) default initial head values, (3) specification of time dependent prescribed boundary conditions, (4) computation and printout of Darcy velocity components and water phase saturation at element centroids, (5) water flow balance computation, and (6) printout control options.

The third problem (Section 10.4) was chosen to demonstrate the code options related to solute transport modeling in a single phase variably saturated flow system. This transport problem corresponds to the flow problem of Section 10.3. Options included for transport modeling are: (1) automatic mesh generation, (2) default initial contamination value, (3) option

to read time varying velocities and water saturation values from the preceding flow simulation via an external binary file (TAPE 9), and (4) specification of prescribed boundary conditions and printout control options.

The fourth problem (Section 10.5) was selected to demonstrate how to simulate three-phase flow using the SAMFT1D code. The options used for input and output are: (1) automatic mesh generation, (2) automatic time stepping scheme, (3) initialization of primary variables using default initial conditions, (4) entry of tabulated relative permeability and capillary pressure curves, (5) specification of boundary conditions with both flux and pressure prescribed on the surface boundary, (6) mass balance computation for the two liquid phases, and (7) printout control options.

The fifth problem (Section 10.6) was provided to show how to simulate multiphase solute transport. The options used are: (1) automatic mesh generation, (2) default nonuniform initial conditions, (3) use of Darcy velocities and saturations of the three phases from the preceding flow simulation via an external file (TAPE9), (4) input of solute properties under multiphase condition, (5) specification of the third type boundary condition at the inlet, and (6) printout control options.

10.2 SINGLE-PHASE HYSTERESIS FLOW SIMULATION PROBLEM

10.2.1 Input Data

This sample problem concerns transient drainage and infiltration in a one-dimensional soil column with hysteresis effects (See Section 4.2.4 for problem description). The input data file is shown in Table 10.2.1. The 60 cm tall soil column is discretized into 60 elements with equal

spacing. The initial condition is given in terms of water saturation. It should be noted that in the input file the hydraulic conductivity, rather than the intrinsic permeability is given. Normally, SAMFT1D expects input values of permeability and initial pressures, and converts these to conductivity and pressure heads, respectively. To expedite the conversion, the values for the fluid density, viscosity and gravitational acceleration are all set to 1. The boundary condition at the soil bottom boundary (node 61) is a prescribed time varying pressure. The time variation is given in input records 15B and 15C.

10.2.2. Output

The main output file for the transient drainage and infiltration problem with hysteresis is listed in Table 10.2.2. This output file contains the following information:

1) Summary of input control parameters;

2) List of automatic time step generation parameters;

3) Summary of flow domain geometry, material properties and grids;

4) Summary of prescribed boundary conditions and initial nodal values of the primary variable;

5) For each selected output time value:

   - nodal values of pressure head
   - summary of the flow mass balance
   - element values of saturation
   - element values of Darcy velocity.

6) CPU time for the simulation. Note that the printed value corresponds to execution on a 25 Mhz 80386 computer.

Table 10.2.1 Input Data for the Single-Phase Hysteretic Flow Simulation Problem

```
   1    1                                                                    GROUP 1
SAMFT1D HYSTERESIS FLOW PROBLEM (CM,MIN) - RESULT IN TERMS OF EFF. SAT.     GROUP 2
   1    2    1    1    1    0    1  200   60    1    0    0                 GROUP 3
   0   10    2       0.1      0.005        1.0       0.0       0.0       0.0 GROUP 4
   0    0    0    0    0    1    1    1    0    1    0    0    2    1       GROUP 5
      0.0       1.0       0.01        2.0      130.0                       GROUP 6
   3    2       0.0       0.0                                              GROUP 7A
   1    1       0.0       1.0                                              GROUP 7B
   2    1      60.0       1.0                                              GROUP 7B
    23.56       0.0     0.301        0.0       0.0                         GROUP 9IA
     1.0        1.0       0.0                                              GROUP 9IB
     0.0      5.509    0.0306      6.779       0.0       1.0       1.0       1.0 GROUP 9IC
     1.0     0.0527                                                        GROUP 9IIA
  +1        1.0    1   60    1    1                                        GROUP 9IIB
   1    0       1.0    0                                                   GROUP 11
   1   60    1       60.0                                                  GROUP 12
   0    0    1    0    0                                                   GROUP 13
  61    1   15    0                                                        GROUP 15A
     0.0       7.27      10.54      22.76      26.20      35.17      45.52      54.90 GROUP 15B
    63.67      68.16      72.25      84.41     104.27     124.14     145.65   GROUP 15B
    60.0       50.0       40.0       30.0       20.0       10.0        0.0      -10.0 GROUP 15B
   -18.45     -12.50     -2.50       7.50      17.50      27.50      37.5     GROUP 15C
     68.0      125.0                                                        GROUP 22A
```

Table 10.2.2 Output of the Single-Phase Hysteretic Flow Simulation Problem.

```
PROBLEM IDENTIFICATION NUMBER =    1

PROBLEM TITLE
-------------------------------------------------------------------------------

SAMFT1D HYSTERESIS FLOW PROBLEM (CM,MIN) - RESULT IN TERMS OF EFF. SAT.

-------------------------------------------------------------------------------


PROBLEM SPECIFICATION PARAMETERS
--------------------------------
MODEL OPTION PARAMETER ...................(IMODL) =    1
  NOTE:  IMODL = 0 FOR SOLUTE TRANSPORT ONLY
               = 1 FOR FLUID FLOW ONLY
               = 2 FOR COUPLED FLOW AND TRANSPORT
TOTAL NUMBER OF FLUID PHASES..... (NTPHAS) =    2
NUMBER OF ACTIVE FLUID PHASES.... (NMPHAS) =    1
HYSTERESIS CONSIDERATION (1=YES,0=NO).....(IHYST) =    1
TOTAL NUMBER OF PRIMARY DEPENDENT VARIABLES(NVAR) =    1
STEADY STATE SIMULATION(1=YES, 0=NO)......(ISSTA) =    0
TIME STEP GENERATION INDEX (1=YES, 0=NO) .(ITSGN) =    1
NUMBER OF TIME STEPS .....................(NTS) =  200
TOTAL NUMBER OF ELEMENTS .................(NE) =   60
NUMBER OF POROUS MATERIALS ...............(NMAT) =    1
SOIL CONSTITUTIVE DATA(0=FUNCTION,1=TABLE)(KPROP) =    0
INITIAL CONDITION NON-UNIFORMITY INDEX ....(NONU) =    0


INPUT / OUTPUT CONTROL PARAMETERS
---------------------------------
VELOCITY/INPUT.........................(NVREAD) =    0
BOUNDARY NODE DATA READ (1=YES, 0=NO)....(IOUTLT) =    0
NUMBER OF NODES FOR WHICH I.C. ARE READ....(NPIN) =    0
OUTPUT REQUIREMENT INDICATOR:
 (0=ALL DATA, 1=NO ELEMENT DATA,
  2=NO DATA, 3=NO MESH AND I.C. DATA.......(IPRD) =    0
UNIT 9 OUTPUT OF VEL / SAT (1=YES, 0=NO).(NVWRIT) =    0
VELOCITY PRINTOUT CONTROL INDEX...........(NVPR) =    1
UNIT 10 AND/OR 11 FOR PLOT (0=NO,>0=YES)..(NPLOT) =    1
TIME STEP INCREMENT FOR OUTPUT PRINT OUT..(NSTEP) =    1
OBSERVATION NODE INDEX..................(IOBSND) =    0
MASS BALANCE TO BE PERFORMED (1=YES,0=NO).(IMBAL) =    1
UNIT 8 OUTPUT OF HEAD/CONC (1=YES, 0=NO).(NOWRIT) =    0
PRINT CHECK OPTION INDEX.................(IPRCHK) =    0
NO. OF SPECIFIED T VALUES FOR PRINTOUT...(NPCORN) =    2

MAX. NUMBER OF NONLINEAR FLOW ITERATIONS.(NITMAX) =   10
CRITERION NO. OF CONVERGENCE TOLERANCE ..(ICONVG) =    2
ICONVG = 1, FOR RELATIVE TOLERANCE,
ICONVG = 2, FOR ABSOLUTE TOLERANCE.
ABSOLUTE PRESSURE TOLERANCE.................(HTOL) =  0.1000E+00
ABSOLUTE SATURATION TOLERANCE...............(STOL) =  0.5000E-02
GRAVITATIONAL ACCELERATION..................(GCONST) =  0.1000E+01
ATMOSPHERE PRESSURE ........................(Patm) =  0.0000E+00
RELATIVE PRESSURE CONVERGENCE TOLERANCE....(RPTOL) =  0.0000E+00
```

```
RELATIVE SATURATION TOLERANCE.....(RSTOL) =  0.0000E+00


TEMPORAL DISCRETIZATION DATA
----------------------------
INITIAL TIME VALUE ..... (TIMA) =  0.0000E+00
VALUE OF FIRST TIME STEP ..... (TIN) =  0.1000E+01
MINIMUM TIME STEP SIZE..... (TMIN) =  0.1000E-01
MAXIMUM TIME STEP SIZE ..... (TMAX) =  0.2000E+01
FINAL TIME VALUE OF THE SIMULATION..... (TEND) =  0.1300E+03


DEFAULT INITIAL CONDITION DATA FOR FLOW PROBLEM
-----------------------------------------------
INITIAL CONDITION IDENTIFIER.....(IDFVAR) =    3
NUMBER OF CONTROL POINTS REQUIRED TO SPECIFY THE
PROFILE OF INITIAL FUNCTION CORRESPONDING TO THE
SPECIFIED VALUE OF IDFVAR.....(NCPONT) =    2
DEFAULT VALUE OF INITIAL SATURATION OF THE NON-
AQUEOUS LIQUID PHASE..... HFDFAL(1) =     0.000
DEFAULT VALUE OF INITIAL PRESSURE OF THE AIR
PHASE.....HIDFAL(2) = 0.000E+00
DEPTH FROM TOP SURFACE OF THE GRID
TO WATER TABLE.....HIDFAL(3) =     0.000


VERTICAL PROFILE FOR INITIAL FUNCTION
-------------------------------------

 CONTROL POINT #     MATERIAL #     VERT. COOR.      FUNCTION VALUE
                                  ( + DOWNWARD )
 ---------------     ----------     -----------      --------------

      1                1            0.0000E+00       1.000
      2                1             60.00           1.000


HYDRAULIC PROPERTIES OF POROUS MEDIA
------------------------------------


MATERIAL NUMBER (I):    1

INTRINSIC PERMEABILITY .....(PROP(I,3)) =  0.2356E+02
POROUS MATRIX COMPRESSIBILITY ..... (PROP(I,4)) =  0.0000E+00
EFFECTIVE POROSITY..... ..... (PROP(I,5)) =  0.3010E+00
IRREDUCIBLE NAPL SATURATION IN N-W ....(SNIRWN(I)) =  0.0000E+00
THRESHOLD NAPL SATURATION.... .....(SNSTR(I)) =  0.0000E+00

FLUID PROPERTIES
----------------

FLUID PHASE NUMBER:    1

REFERENCE DENSITY..... =  0.1000E+01
REFERENCE DYNAMIC VISCOSITY..... =  0.1000E+01
COMPRESSIBILITY ..... =  0.0000E+00

FLUID RETENTION FUNCTIONAL PARAMETERS
-------------------------------------

SOIL MATERIAL NUMBER (I):    1

IRREDUCIBLE WETTING PHASE SATURATION.....PROP(I,7) =  0.0000E+00
EXPONENT INDEX OF REL. PERM. FUNCTION....PROP(I,8) =  0.5509E+01
COEFF. ALPHA.....PROP(I,9) =  0.3060E-01
POWER INDEX BETA.....PROP(I,10) =  0.6779E+01
POWER INDEX GAMMA.....PROP(I,11) =  0.8525E+00
```

```
SURFACE TENSION BETWEEN AIR AND WATER...PROP(I,12) =  0.1000E+01
SURFACE TENSION BETWEEN NAPL AND WATER..PROP(I,13) =  0.1000E+01
SURFACE TENSION BETWEEN AIR AND NAPL....PROP(I,14) =  0.1000E+01

          MAIN WETTING PARAMETERS
          -----------------------
MAXIMUM WETTING SATURATION..... (PROP(I,15)) =  0.1000E+01
COEFF (ALPHA) OF SAT. VS CAPIL. PRES. (PROP(I,16)) =  0.5270E-01


INITIAL HYSTERESIS INDEX AND WATER SATURATION
---------------------------------------------

KHYSTV        SWINTV     STARTING ELEM.    ENDING ELEM.    ENDING ELEM.    ELEM. INCR.

    1     0.100E+01           1               60              1               1


GRID GENERATION PARAMETERS
--------------------------
NUMBER OF SOIL LAYERS.....................(NLAYER) =    1
PARAMETER INDICATING THE GRID TYPE (IBCGR)
(0=MESH-CENTERED (F.E.), 1=BLOCK-CENTERED(F.D.))...=    0
PARAMETER INDICATING GRID ORIENTATION.....(IHORGR) =    0
IHORGR=0 FOR VERTICAL FLOW, IHORGR=1 FOR HORIZONTAL FLOW


LAYERED GRID DATA
-----------------


LAYER NUMBER :    1
------------------
NO. OF ELEMENTS (OR GRID BLOCKS) ..........(NELM) =   60
MATERIAL NUMBER ...........................(IMATL) =    1
LAYER THICKNESS............................(THL) =  0.6000E+02


************************************************
*** MESH-CENTERED FINITE ELEMENT GRID IS USED ***
************************************************
```

NODE	Z-COOR.	NODE	Z-COOR.	NODE	Z-COOR.	NODE	Z-COOR.
1	0.00	2	1.00	3	2.00	4	3.00
5	4.00	6	5.00	7	6.00	8	7.00
9	8.00	10	9.00	11	10.00	12	11.00
13	12.00	14	13.00	15	14.00	16	15.00
17	16.00	18	17.00	19	18.00	20	19.00
21	20.00	22	21.00	23	22.00	24	23.00
25	24.00	26	25.00	27	26.00	28	27.00
29	28.00	30	29.00	31	30.00	32	31.00
33	32.00	34	33.00	35	34.00	36	35.00
37	36.00	38	37.00	39	38.00	40	39.00
41	40.00	42	41.00	43	42.00	44	43.00
45	44.00	46	45.00	47	46.00	48	47.00
49	48.00	50	49.00	51	50.00	52	51.00
53	52.00	54	53.00	55	54.00	56	55.00
57	56.00	58	57.00	59	58.00	60	59.00
61	60.00						

```
BOUNDARY CONDITION DATA
-----------------------
```

```
NO. OF STEADY DIRICHLET BOUNDARY CONDITIONS....(NBTO) =    0
NO. OF STEADY FLUX BOUNDARY CONDITIONS..... (NDFLUX) =    0
NO. OF TRANSIENT DIRICHLET BOUNDARY CONDITIONS(NBHVAR)=   1
NO. OF TRANSIENT FLUX BOUNDARY CONDITIONS... (NBFVAR) =    0
BOUNDARY SPECIFICATION # OF SURFACE NODE.....(NBCND1) =    0
BOUNDARY SPECIFICATION # OF BOTTOM  NODE.....(NBCNDN) =    0


TRANSIENT DIRICHLET BOUNDARY CONDITIONS
---------------------------------------


TIME DEPENDENT DIRICHLET B. C. FOR  NODE NO.    61     VALUE OF MDEGBT(I)      1
-------------------------------------------------------------------------------
NUMBER OF CONTROL POINTS IN THE TIME GRAPH =   15
TEMPORAL VARIATION (0=CONTINUOUS, 1=STEP)  =    0

TIME VERSUS PRESCRIBED PHASE PRESSURE
-------------------------------------
     (TIME)          (PRESSURE)

  0.0000E+00          60.00
    7.270             50.00
    10.54             40.00
    22.76             30.00
    26.20             20.00
    35.17             10.00
    45.52          0.0000E+00
    54.90            -10.00
    63.67            -18.45
    68.16            -12.50
    72.25            -2.500
    84.41             7.500
    104.3             17.50
    124.1             27.50
    145.7             37.50


*** DEFAULT INITIAL CONDITION ***
---------------------------------


INITIAL VALUES OF DEPENDENT VARIABLE #   1
-----------------------------------------
```

NODE NUMBER	DEPENDENT VARIABLE	NODE NUMBER	DEPENDENT VARIABLE	NODE NUMBER	DEPENDENT VARIABLE	NODE NUMBER	DEPENDENT VARIABLE	NODE NUMBER	DEPENDENT VARIABLE
1	1.000	2	1.000	3	1.000	4	1.000	5	1.000
6	1.000	7	1.000	8	1.000	9	1.000	10	1.000
11	1.000	12	1.000	13	1.000	14	1.000	15	1.000
16	1.000	17	1.000	18	1.000	19	1.000	20	1.000
21	1.000	22	1.000	23	1.000	24	1.000	25	1.000
26	1.000	27	1.000	28	1.000	29	1.000	30	1.000
31	1.000	32	1.000	33	1.000	34	1.000	35	1.000
36	1.000	37	1.000	38	1.000	39	1.000	40	1.000
41	1.000	42	1.000	43	1.000	44	1.000	45	1.000
46	1.000	47	1.000	48	1.000	49	1.000	50	1.000
51	1.000	52	1.000	53	1.000	54	1.000	55	1.000
56	1.000	57	1.000	58	1.000	59	1.000	60	1.000
61	1.000								

```
LIST OF TIME VALUES FOR PRINTING SIMULATION RESULT
--------------------------------------------------
```

0.68000E+02 0.12500E+03

****
*** ELAPSED SIMULATION TIME : 68.00 ***
****

CUMULATIVE NUMBER OF COMPUTATIONAL TIME STEPS : 36

CURRENT VALUE OF COMPUTATIONAL TIME STEP (DT) : 0.20000E+01

* NODAL PRESSURE VALUES *

NODE	PRESSURE	NODE	PRESSURE	NODE	PRESSURE	NODE	PRESSURE	NODE	PRESSURE
1	-45.14	2	-44.37	3	-43.84	4	-43.43	5	-43.09
6	-42.81	7	-42.56	8	-42.35	9	-42.15	10	-41.97
11	-41.81	12	-41.65	13	-41.51	14	-41.38	15	-41.25
16	-41.13	17	-41.02	18	-40.91	19	-40.80	20	-40.70
21	-40.60	22	-40.50	23	-40.41	24	-40.31	25	-40.22
26	-40.13	27	-40.04	28	-39.95	29	-39.85	30	-39.73
31	-39.59	32	-39.39	33	-39.12	34	-38.74	35	-38.24
36	-37.59	37	-36.77	38	-35.82	39	-34.80	40	-33.76
41	-32.72	42	-31.68	43	-30.65	44	-29.62	45	-28.60
46	-27.58	47	-26.57	48	-25.56	49	-24.55	50	-23.54
51	-22.54	52	-21.53	53	-20.53	54	-19.52	55	-18.52
56	-17.52	57	-16.51	58	-15.51	59	-14.51	60	-13.50
61	-12.50								

*** VOLUMETRIC FLOW BALANCE INFORMATION AT TIME = 0.6977E+02***

SUMMARY OF FLOW MASS BALANCE

FLUID FLUX VALUE AT FIRST NODE = 0.1238E-04
FLUID FLUX VALUE AT LAST NODE = 0.1609E+00
NET VALUE OF FLUID FLUX = 0.1609E+00
NET RATE OF VOLUMETRIC STORAGE = 0.1617E+00
FLOW BALANCE ERROR = -0.7802E-03
CUMULATIVE VOLUMETRIC STORAGE = -0.9277E+01
CUMULATIVE INFLOW VOLUME = -0.1401E-01
CUMULATIVE OUTFLOW VOLUME = -0.9206E+01

*** LIST OF PARTIALLY SATURATED ELEMENTS ***

ELEM.	SAT. VALUE	ELEM.	SAT. VALUE	ELEM.	SAT. VALUE	ELEM.	SAT. VALUE	ELEM.	SAT. VALUE
1	0.1478	2	0.1593	3	0.1682	4	0.1756	5	0.1820
6	0.1877	7	0.1928	8	0.1976	9	0.2019	10	0.2060
11	0.2098	12	0.2135	13	0.2169	14	0.2202	15	0.2234
16	0.2265	17	0.2295	18	0.2323	19	0.2352	20	0.2379
21	0.2406	22	0.2433	23	0.2460	24	0.2486	25	0.2512
26	0.2539	27	0.2566	28	0.2594	29	0.2626	30	0.2658
31	0.2698	32	0.2752	33	0.2832	34	0.2913	35	0.2994
36	0.3105	37	0.3256	38	0.3460	39	0.3637	40	0.3839

41	0.4085	42	0.4380	43	0.4728	44	0.5125	45	0.5565
46	0.6038	47	0.6531	48	0.7029	49	0.7516	50	0.7979
51	0.8404	52	0.8780	53	0.9100	54	0.9362	55	0.9566
56	0.9718	57	0.9825	58	0.9895	59	0.9940	60	0.9967

*** ELEMENTAL DARCY VELOCITY ***

ELEMENT	VELOCITY	ELEMENT	VELOCITY	ELEMENT	VELOCITY	ELEMENT	VELOCITY
1	1.355E-04	2	4.180E-04	3	7.131E-04	4	1.020E-03
5	1.339E-03	6	1.668E-03	7	2.008E-03	8	2.357E-03
9	2.716E-03	10	3.084E-03	11	3.462E-03	12	3.849E-03
13	4.245E-03	14	4.652E-03	15	5.068E-03	16	5.495E-03
17	5.933E-03	18	6.383E-03	19	6.844E-03	20	7.317E-03
21	7.803E-03	22	8.301E-03	23	8.810E-03	24	9.325E-03
25	9.837E-03	26	1.033E-02	27	1.078E-02	28	1.115E-02
29	1.135E-02	30	1.116E-02	31	9.926E-03	32	6.143E-03
33	-2.166E-03	34	-2.721E-03	35	-3.792E-03	36	-5.265E-03
37	-7.186E-03	38	-9.599E-03	39	-1.259E-02	40	-1.629E-02
41	-2.081E-02	42	-2.630E-02	43	-3.286E-02	44	-4.059E-02
45	-4.953E-02	46	-5.967E-02	47	-7.089E-02	48	-8.296E-02
49	-9.548E-02	50	-0.108	51	-0.120	52	-0.130
53	-0.139	54	-0.146	55	-0.152	56	-0.155
57	-0.158	58	-0.159	59	-0.160	60	-0.161

****
*** ELAPSED SIMULATION TIME : 125.0 ***
****

CUMULATIVE NUMBER OF COMPUTATIONAL TIME STEPS : 64

CURRENT VALUE OF COMPUTATIONAL TIME STEP (DT) : 0.20000E+01

* NODAL PRESSURE VALUES *

NODE	PRESSURE	NODE	PRESSURE	NODE	PRESSURE	NODE	PRESSURE	NODE	PRESSURE
1	-39.90	2	-38.52	3	-36.73	4	-34.72	5	-32.61
6	-30.50	7	-28.51	8	-26.75	9	-25.21	10	-23.86
11	-22.64	12	-21.52	13	-20.44	14	-19.39	15	-18.36
16	-17.34	17	-16.33	18	-15.32	19	-14.31	20	-13.30
21	-12.30	22	-11.29	23	-10.29	24	-9.284	25	-8.279
26	-7.274	27	-6.269	28	-5.264	29	-4.259	30	-3.255
31	-2.250	32	-1.245	33	-0.2402	34	0.7646	35	1.769
36	2.774	37	3.779	38	4.784	39	5.789	40	6.793
41	7.798	42	8.803	43	9.808	44	10.81	45	11.82
46	12.82	47	13.83	48	14.83	49	15.84	50	16.84
51	17.85	52	18.85	53	19.86	54	20.86	55	21.87
56	22.87	57	23.88	58	24.88	59	25.88	60	26.89
61	27.89								

*** VOLUMETRIC FLOW BALANCE INFORMATION AT TIME = 0.1258E+03***

SUMMARY OF FLOW MASS BALANCE

FLUID FLUX VALUE AT FIRST NODE = 0.7992E-06
FLUID FLUX VALUE AT LAST NODE = 0.1114E+00
NET VALUE OF FLUID FLUX = 0.1114E+00
NET RATE OF VOLUMETRIC STORAGE = 0.1127E+00
FLOW BALANCE ERROR = -0.1344E-02
CUMULATIVE VOLUMETRIC STORAGE = -0.2027E+01
CUMULATIVE INFLOW VOLUME = -0.1395E-01
CUMULATIVE OUTFLOW VOLUME = -0.2019E+01

*** LIST OF PARTIALLY SATURATED ELEMENTS ***

ELEM.	SAT. VALUE	ELEM.	SAT. VALUE	ELEM.	SAT. VALUE	ELEM.	SAT. VALUE	ELEM.	SAT. VALUE
1	0.1351	2	0.1494	3	0.1640	4	0.1806	5	0.2010
6	0.2271	7	0.2597	8	0.2987	9	0.3436	10	0.3940
11	0.4507	12	0.5128	13	0.5800	14	0.6501	15	0.7196
16	0.7852	17	0.8429	18	0.8908	19	0.9278	20	0.9547
21	0.9731	22	0.9849	23	0.9920	24	0.9961	25	0.9982
26	0.9993	27	0.9997	28	0.9999	29	1.0000	30	1.0000
31	1.0000	32	1.0000	33	1.0000	34	1.0000	35	1.0000
36	1.0000	37	1.0000	38	1.0000	39	1.0000	40	1.0000
41	1.0000	42	1.0000	43	1.0000	44	1.0000	45	1.0000
46	1.0000	47	1.0000	48	1.0000	49	1.0000	50	1.0000
51	1.0000	52	1.0000	53	1.0000	54	1.0000	55	1.0000
56	1.0000	57	1.0000	58	1.0000	59	1.0000	60	1.0000

*** ELEMENTAL DARCY VELOCITY ***

ELEMENT	VELOCITY	ELEMENT	VELOCITY	ELEMENT	VELOCITY	ELEMENT	VELOCITY
1	-1.584E-04	2	-5.877E-04	3	-1.260E-03	4	-2.389E-03
5	-4.318E-03	6	-7.450E-03	7	-1.196E-02	8	-1.758E-02
9	-2.393E-02	10	-3.085E-02	11	-3.839E-02	12	-4.668E-02
13	-5.566E-02	14	-6.510E-02	15	-7.455E-02	16	-8.342E-02
17	-9.121E-02	18	-9.758E-02	19	-0.102	20	-0.106
21	-0.108	22	-0.110	23	-0.110	24	-0.111
25	-0.111	26	-0.111	27	-0.111	28	-0.111
29	-0.111	30	-0.111	31	-0.111	32	-0.111
33	-0.111	34	-0.111	35	-0.111	36	-0.111
37	-0.111	38	-0.111	39	-0.111	40	-0.111
41	-0.111	42	-0.111	43	-0.111	44	-0.111
45	-0.111	46	-0.111	47	-0.111	48	-0.111
49	-0.111	50	-0.111	51	-0.111	52	-0.111
53	-0.111	54	-0.111	55	-0.111	56	-0.111
57	-0.111	58	-0.111	59	-0.111	60	-0.111

***** SAMFT1D HAS SOLVED THE PROBLEM *****

****
*** CPU TIME USED: 30.71 SECS. ***
****

10.3 SINGLE-PHASE FLOW SIMULATION PROBLEM

10.3.1 Input Data

This example problem involves transient infiltration in a layered root zone. The input data file is shown in Table 10.3.1. The input group identification numbers depicted with each input record correspond to the input groups as discussed in Section 8.3. The soil profile is discretized into 15 elements. The first layer extends from the soil surface to a depth of 10 cm and contains 2 elements. The second layer extends to a depth of 40 cm and contains 6 elements. The third layer extends to a depth of 100 cm and contains 7 elements. It should be noted that in the input file the hydraulic conductivity, rather than the intrinsic permeability for each layer is given, and the initial condition is given in terms of pressure head. Normally, SAMFT1D expects input values of permeability and initial pressures, and converts these to conductivity and pressure heads, respectively. To expedite the conversion, the values for the fluid density, viscosity and gravitational acceleration are all set to 1. The boundary condition at the bottom node (node 16) is set to a constant value of -100 cm. The boundary condition at the soil surface (node 1) is a prescribed time varying infiltration rate. The time variation is given in input records 16B and 16C.

10.3.2 Output

The main output file for the root zone infiltration problem is listed in Table 10.3.2. This output file contains the following information:

1) Summary of input control parameters;

2) List of automatic time step generation parameters;

Table 10.3.1 Input Data for the Single-Phase Flow Simulation Problem

```
  1    1                                                                  GROUP.1
SAMFT1D SINGLE PHASE MODULE: ROOTZONE INFILTR (INPUT HYDR. COND. & PR. HEAD)  ...2
  1    2    1    0    1    0    1    5   15    3    0                      ...3
  0   10    2        0.1       0.0       1.0       0.0       0.0          ...4
  0    0    0    0    1    1    0    1    0    1    0    0    0    1       ...5
     0.0       0.5       1.0       0.5   1.00E09                          .6A1
  1    4       0.0       0.0       0.0                                    ..7A
  1    3       0.0    -100.0                                              ..7B
  2    2      10.0    -100.0                                              ....
  3    1      40.0    -100.0                                              ....
  4    1     100.0    -100.0                                              ....
   350.0       0.0       0.41                                            ..9A
    25.0       0.0       0.43                                            ....
    10.8       0.0       0.45                                            ....
     1.0       1.0       0.0                                             ..9B
 0.0574       1.0     0.124      2.28    0.5164       0.0       0.0       0.0 ..9C
 0.0774       1.0     0.036      1.56    0.3590       0.0       0.0       0.0 ..9C
 0.0675       1.0     0.020      1.41    0.2908       0.0       0.0       0.0 ..9C
  3    0       1.0     0                                                  ..11
  1    2    3       10.0                                                  ..12
  2    6    2       30.0                                                  ....
  3    7    1       60.0                                                  ....
  1    0    0    1                                                        ..13
 16    1    -100.0                                                        ..14
  1    1    6                                                             .16A
     0.0       1.0       2.0       3.0       4.0      50.0                .16B
     0.0      12.5      10.0       0.0       0.0       0.0                .16C
```

Table 10.3.2 Output for the Single-Phase Flow Simulation Problem.

```
PROBLEM IDENTIFICATION NUMBER =    1

PROBLEM TITLE
-------------------------------------------------------------------------------

 SAMFT1D SINGLE PHASE MODULE: ROOTZONE INFILTR (INPUT HYDR. COND. & PR. HEAD)

-------------------------------------------------------------------------------



PROBLEM SPECIFICATION PARAMETERS
--------------------------------
MODEL OPTION PARAMETER ...................(IMODL) =    1
  NOTE:  IMODL = 0 FOR SOLUTE TRANSPORT ONLY
               = 1 FOR FLUID FLOW ONLY
               = 2 FOR COUPLED FLOW AND TRANSPORT
TOTAL NUMBER OF FLUID PHASES..... (NTPHAS) =    2
NUMBER OF ACTIVE FLUID PHASES..... (NMPHAS) =    1
HYSTERESIS CONSIDERATION (1=YES,0=NO).....(IHYST) =    0
TOTAL NUMBER OF PRIMARY DEPENDENT VARIABLES(NVAR) =    1
STEADY STATE SIMULATION(1=YES, 0=NO)......(ISSTA) =    0
TIME STEP GENERATION INDEX (1=YES, 0=NO) .(ITSGN) =    1
NUMBER OF TIME STEPS .....................(NTS) =    5
TOTAL NUMBER OF ELEMENTS .................(NE) =   15
NUMBER OF POROUS MATERIALS ...............(NMAT) =    3
SOIL CONSTITUTIVE DATA(0=FUNCTION,1=TABLE)(KPROP) =    0
INITIAL CONDITION NON-UNIFORMITY INDEX ....(NONU) =    0


INPUT / OUTPUT CONTROL PARAMETERS
---------------------------------
VELOCITY/INPUT.........................(NVREAD) =    0
BOUNDARY NODE DATA READ (1=YES, 0=NO)....(IOUTLT) =    0
NUMBER OF NODES FOR WHICH I.C. ARE READ....(NPIN) =    0
OUTPUT REQUIREMENT INDICATOR:
 (0=ALL DATA, 1=NO ELEMENT DATA,
  2=NO DATA, 3=NO MESH AND I.C. DATA.......(IPRD) =    0
UNIT 9 OUTPUT OF VEL / SAT (1=YES, 0=NO).(NVWRIT) =    1
VELOCITY PRINTOUT CONTROL INDEX.............(NVPR) =    1
UNIT 10 AND/OR 11 FOR PLOT (0=NO,>0=YES)..(NPLOT) =    0
TIME STEP INCREMENT FOR OUTPUT PRINT OUT..(NSTEP) =    1
OBSERVATION NODE INDEX...................(IOBSND) =    0
MASS BALANCE TO BE PERFORMED (1=YES,0=NO).(IMBAL) =    1
UNIT 8 OUTPUT OF HEAD/CONC (1=YES, 0=NO).(NOWRIT) =    0
PRINT CHECK OPTION INDEX.................(IPRCHK) =    0
NO. OF SPECIFIED T VALUES FOR PRINTOUT...(NPCORN) =    0

MAX. NUMBER OF NONLINEAR FLOW ITERATIONS.(NITMAX) =   10
CRITERION NO. OF CONVERGENCE TOLERANCE ..(ICONVG) =    2
ICONVG = 1, FOR RELATIVE TOLERANCE,
ICONVG = 2, FOR ABSOLUTE TOLERANCE.
ABSOLUTE PRESSURE TOLERANCE.................(HTOL) =  0.1000E+00
ABSOLUTE SATURATION TOLERANCE...............(STOL) =  0.1000E-02
GRAVITATIONAL ACCELERATION..................(GCONST) =  0.1000E+01
ATMOSPHERE PRESSURE ........................(Patm) =  0.0000E+00
RELATIVE PRESSURE CONVERGENCE TOLERANCE....(RPTOL) =  0.0000E+00
```

```
RELATIVE SATURATION TOLERANCE.............(RSTOL) =  0.0000E+00


TEMPORAL DISCRETIZATION DATA
----------------------------
INITIAL TIME VALUE ..................... (TIMA) =  0.0000E+00
VALUE OF FIRST TIME STEP ..............  (TIN) =  0.5000E+00
MINIMUM TIME STEP SIZE.................. (TMIN) =  0.1000E+01
MAXIMUM TIME STEP SIZE ................. (TMAX) =  0.5000E+00
FINAL TIME VALUE OF THE SIMULATION..... (TEND) =  0.1000E+10


DEFAULT INITIAL CONDITION DATA FOR FLOW PROBLEM
-----------------------------------------------
INITIAL CONDITION IDENTIFIER.............(IDFVAR) =    1
NUMBER OF CONTROL POINTS REQUIRED TO SPECIFY THE
PROFILE OF INITIAL FUNCTION CORRESPONDING TO THE
SPECIFIED VALUE OF IDFVAR................(NCPONT) =    4
DEFAULT VALUE OF INITIAL SATURATION OF THE NON-
AQUEOUS LIQUID PHASE..................... HFDFAL(1) =     0.000
DEFAULT VALUE OF INITIAL PRESSURE OF THE AIR
PHASE.....................................HIDFAL(2) = 0.000E+00
DEPTH FROM TOP SURFACE OF THE GRID
TO WATER TABLE............................HIDFAL(3) =     0.000


VERTCAL PROFILE FOR INITIAL FUNCTION
------------------------------------

 CONTROL POINT #     MATERIAL #     VERT. COOR.      FUNCTION VALUE
                                  ( + DOWNWARD )
 ---------------     ----------     -----------      --------------

      1                3             0.0000E+00      -100.0
      2                2              10.00          -100.0
      3                1              40.00          -100.0
      4                1              100.0          -100.0


HYDRAULIC PROPERTIES OF POROUS MEDIA
------------------------------------


MATERIAL NUMBER (I):    1

INTRINSIC PERMEABILITY .................(PROP(I,3)) =  0.3500E+03
POROUS MATRIX COMPRESSIBILITY ........ (PROP(I,4)) =  0.0000E+00
EFFECTIVE POROSITY..... ...... (PROP(I,5)) =  0.4100E+00
IRREDUCIBLE NAPL SATURATION IN N-W ....(SNIRWN(I)) =  0.0000E+00
THRESHOLD NAPL SATURATION.... ..........(SNSTR(I)) =  0.0000E+00

MATERIAL NUMBER (I):    2

INTRINSIC PERMEABILITY .................(PROP(I,3)) =  0.2500E+02
POROUS MATRIX COMPRESSIBILITY ........ (PROP(I,4)) =  0.0000E+00
EFFECTIVE POROSITY..... ...... (PROP(I,5)) =  0.4300E+00
IRREDUCIBLE NAPL SATURATION IN N-W ....(SNIRWN(I)) =  0.0000E+00
THRESHOLD NAPL SATURATION.... ..........(SNSTR(I)) =  0.0000E+00

MATERIAL NUMBER (I):    3

INTRINSIC PERMEABILITY .................(PROP(I,3)) =  0.1080E+02
POROUS MATRIX COMPRESSIBILITY ........ (PROP(I,4)) =  0.0000E+00
EFFECTIVE POROSITY..... ...... (PROP(I,5)) =  0.4500E+00
IRREDUCIBLE NAPL SATURATION IN N-W ....(SNIRWN(I)) =  0.0000E+00
THRESHOLD NAPL SATURATION.... ..........(SNSTR(I)) =  0.0000E+00

FLUID PROPERTIES
```

```
---------------

FLUID PHASE NUMBER:    1

REFERENCE DENSITY..................................... =  0.1000E+01
REFERENCE DYNAMIC VISCOSITY........................... =  0.1000E+01
COMPRESSIBILITY ...................................... =  0.0000E+00

FLUID RETENTION FUNCTIONAL PARAMETERS
-------------------------------------

SOIL MATERIAL NUMBER (I):    1

IRREDUCIBLE WETTING PHASE SATURATION.....PROP(I,7) =  0.5740E-01
EXPONENT INDEX OF REL. PERM. FUNCTION....PROP(I,8) =  0.1000E+01
COEFF. ALPHA.............................PROP(I,9) =  0.1240E+00
POWER INDEX BETA.........................PROP(I,10) =  0.2280E+01
POWER INDEX GAMMA........................PROP(I,11) =  0.5164E+00
SURFACE TENSION BETWEEN AIR AND WATER...PROP(I,12) =  0.0000E+00
SURFACE TENSION BETWEEN NAPL AND WATER..PROP(I,13) =  0.0000E+00
SURFACE TENSION BETWEEN AIR AND NAPL....PROP(I,14) =  0.0000E+00

SOIL MATERIAL NUMBER (I):    2

IRREDUCIBLE WETTING PHASE SATURATION.....PROP(I,7) =  0.7740E-01
EXPONENT INDEX OF REL. PERM. FUNCTION....PROP(I,8) =  0.1000E+01
COEFF. ALPHA.............................PROP(I,9) =  0.3600E-01
POWER INDEX BETA.........................PROP(I,10) =  0.1560E+01
POWER INDEX GAMMA........................PROP(I,11) =  0.3590E+00
SURFACE TENSION BETWEEN AIR AND WATER...PROP(I,12) =  0.0000E+00
SURFACE TENSION BETWEEN NAPL AND WATER..PROP(I,13) =  0.0000E+00
SURFACE TENSION BETWEEN AIR AND NAPL....PROP(I,14) =  0.0000E+00

SOIL MATERIAL NUMBER (I):    3

IRREDUCIBLE WETTING PHASE SATURATION.....PROP(I,7) =  0.6750E-01
EXPONENT INDEX OF REL. PERM. FUNCTION....PROP(I,8) =  0.1000E+01
COEFF. ALPHA.............................PROP(I,9) =  0.2000E-01
POWER INDEX BETA.........................PROP(I,10) =  0.1410E+01
POWER INDEX GAMMA........................PROP(I,11) =  0.2908E+00
SURFACE TENSION BETWEEN AIR AND WATER...PROP(I,12) =  0.0000E+00
SURFACE TENSION BETWEEN NAPL AND WATER..PROP(I,13) =  0.0000E+00
SURFACE TENSION BETWEEN AIR AND NAPL....PROP(I,14) =  0.0000E+00


GRID GENERATION PARAMETERS
--------------------------
NUMBER OF SOIL LAYERS.....................(NLAYER) =    3
PARAMETER INDICATING THE GRID TYPE (IBCGR)
(0=MESH-CENTERED (F.E.), 1=BLOCK-CENTERED(F.D.))...=    0
PARAMETER INDICATING GRID ORIENTATION.....(IHORGR) =    0
IHORGR=0 FOR VERTICAL FLOW, IHORGR=1 FOR HORIZONTAL FLOW



LAYERED GRID DATA
-----------------


LAYER NUMBER :    1
------------------
NO. OF ELEMENTS (OR GRID BLOCKS) ..........(NELM) =    2
MATERIAL NUMBER ...........................(IMATL) =    3
LAYER THICKNESS............................(THL) =  0.1000E+02

LAYER NUMBER :    2
------------------
NO. OF ELEMENTS (OR GRID BLOCKS) ..........(NELM) =    6
MATERIAL NUMBER ...........................(IMATL) =    2
```

```
LAYER THICKNESS.............................(THL) =  0.3000E+02

LAYER NUMBER :    3
------------------
NO. OF ELEMENTS (OR GRID BLOCKS) ..........(NELM) =    7
MATERIAL NUMBER ............................(IMATL) =    1
LAYER THICKNESS.............................(THL) =  0.6000E+02



************************************************
*** MESH-CENTERED FINITE ELEMENT GRID IS USED ***
************************************************
```

NODE	Z-COOR.	NODE	Z-COOR.	NODE	Z-COOR.	NODE	Z-COOR.
1	0.00	2	5.00	3	10.00	4	15.00
5	20.00	6	25.00	7	30.00	8	35.00
9	40.00	10	48.57	11	57.14	12	65.71
13	74.29	14	82.86	15	91.43	16	100.00

ELEMENT	MATL. NO.	ELEMENT	MATL. NO.	ELEMENT	MATL. NO.	ELEMENT	MATL. NO.
1	3	2	3	3	2	4	2
5	2	6	2	7	2	8	2
9	1	10	1	11	1	12	1
13	1	14	1	15	1		

```
BOUNDARY CONDITION DATA
-----------------------

NO. OF STEADY DIRICHLET BOUNDARY CONDITIONS....(NBTO) =    1
NO. OF STEADY FLUX BOUNDARY CONDITIONS..... (NDFLUX) =    0
NO. OF TRANSIENT DIRICHLET BOUNDARY CONDITIONS(NBHVAR)=    0
NO. OF TRANSIENT FLUX BOUNDARY CONDITIONS... (NBFVAR) =    1
BOUNDARY SPECIFICATION # OF SURFACE NODE.....(NBCND1) =    0
BOUNDARY SPECIFICATION # OF BOTTOM  NODE.....(NBCNDN) =    0


STEADY-STATE DIRICHLET BOUNDARY CONDITIONS
------------------------------------------
```

INDEX	NODE NO.	MDEGB(I)	PRESCRIBED VALUE
1	16	1	-100.0

```
TRANSIENT FLUX BOUNDARY CONDITIONS
----------------------------------


TIME DEPENDENT FLUX B. C. FOR  NODE NO.    1     VALUE OF MDEGFT(I)     1
-------------------------------------------------------------------------
NUMBER OF CONTROL POINTS IN THE TIME GRAPH =    6
TEMPORAL VARIATION (0=CONTINUOUS, 1=STEP)  =    0


    TIME VERSUS PRESCRIBED FLUID FLUXES
    -----------------------------------
```

(TIME)	(FLUID FLUXES)
0.0000E+00	0.0000E+00
1.000	12.50
2.000	10.00
3.000	0.0000E+00
4.000	0.0000E+00
50.00	0.0000E+00

*** DEFAULT INITIAL CONDITION ***

INITIAL VALUES OF DEPENDENT VARIABLE # 1

NODE NUMBER	DEPENDENT VARIABLE	NODE NUMBER	DEPENDENT VARIABLE	NODE NUMBER	DEPENDENT VARIABLE	NODE NUMBER	DEPENDENT VARIABLE	NODE NUMBER	DEPENDENT VARIABLE
1	-100.0	2	-100.0	3	-100.0	4	-100.0	5	-100.0
6	-100.0	7	-100.0	8	-100.0	9	-100.0	10	-100.0
11	-100.0	12	-100.0	13	-100.0	14	-100.0	15	-100.0
16	-100.0								

****
*** ELAPSED SIMULATION TIME : 0.5000 ***
****

CUMULATIVE NUMBER OF COMPUTATIONAL TIME STEPS : 1

CURRENT VALUE OF COMPUTATIONAL TIME STEP (DT) : 0.50000E+00

* NODAL PRESSURE VALUES *

NODE	PRESSURE	NODE	PRESSURE	NODE	PRESSURE	NODE	PRESSURE	NODE	PRESSURE
1	-135.7	2	-135.4	3	-135.3	4	-133.8	5	-132.3
6	-131.0	7	-129.7	8	-128.6	9	-127.5	10	-124.0
11	-120.4	12	-116.7	13	-112.8	14	-108.7	15	-104.4
16	-100.0								

*** VOLUMETRIC FLOW BALANCE INFORMATION AT TIME = 0.5000E+00***

SUMMARY OF FLOW MASS BALANCE

FLUID FLUX VALUE AT FIRST NODE	= 0.6253E+01
FLUID FLUX VALUE AT LAST NODE	= -0.8454E+01
NET VALUE OF FLUID FLUX	= -0.2201E+01
NET RATE OF VOLUMETRIC STORAGE	= -0.2206E+01
FLOW BALANCE ERROR	= 0.4927E-02
CUMULATIVE VOLUMETRIC STORAGE	= -0.1103E+01
CUMULATIVE INFLOW VOLUME	= 0.3126E+01
CUMULATIVE OUTFLOW VOLUME	= -0.4227E+01

*** LIST OF PARTIALLY SATURATED ELEMENTS ***

ELEM.	SAT. VALUE	ELEM.	SAT. VALUE	ELEM.	SAT. VALUE	ELEM.	SAT. VALUE	ELEM.	SAT. VALUE
1	0.6488	2	0.6490	3	0.4477	4	0.4498	5	0.4518
6	0.4538	7	0.4556	8	0.4572	9	0.0945	10	0.0958
11	0.0972	12	0.0987	13	0.1005	14	0.1025	15	0.1060

*** ELEMENTAL DARCY VELOCITY ***

ELEMENT	VELOCITY	ELEMENT	VELOCITY	ELEMENT	VELOCITY	ELEMENT	VELOCITY
1	6.38	2	6.65	3	6.91	4	7.17
5	7.41	6	7.65	7	7.87	8	8.09
9	8.17	10	8.25	11	8.31	12	8.37
13	8.41	14	8.44	15	8.45		

****
*** ELAPSED SIMULATION TIME : 1.000 ***
****

CUMULATIVE NUMBER OF COMPUTATIONAL TIME STEPS : 2

CURRENT VALUE OF COMPUTATIONAL TIME STEP (DT) : 0.50000E+00

* NODAL PRESSURE VALUES *

NODE	PRESSURE	NODE	PRESSURE	NODE	PRESSURE	NODE	PRESSURE	NODE	PRESSURE
1	-107.5	2	-111.1	3	-114.7	4	-115.2	5	-115.8
6	-116.2	7	-116.7	8	-117.1	9	-117.5	10	-115.4
11	-113.3	12	-111.0	13	-108.5	14	-105.8	15	-103.0
16	-100.0								

*** VOLUMETRIC FLOW BALANCE INFORMATION AT TIME = 0.1000E+01***

SUMMARY OF FLOW MASS BALANCE

FLUID FLUX VALUE AT FIRST NODE = 0.1250E+02
FLUID FLUX VALUE AT LAST NODE = -0.1148E+02
NET VALUE OF FLUID FLUX = 0.1022E+01
NET RATE OF VOLUMETRIC STORAGE = 0.1018E+01
FLOW BALANCE ERROR = 0.4446E-02

CUMULATIVE VOLUMETRIC STORAGE = -0.5943E+00
CUMULATIVE INFLOW VOLUME = 0.9379E+01
CUMULATIVE OUTFLOW VOLUME = -0.9968E+01

*** LIST OF PARTIALLY SATURATED ELEMENTS ***

ELEM.	SAT. VALUE	ELEM.	SAT. VALUE	ELEM.	SAT. VALUE	ELEM.	SAT. VALUE	ELEM.	SAT. VALUE
1	0.6900	2	0.6839	3	0.4787	4	0.4777	5	0.4768
6	0.4760	7	0.4753	8	0.4746	9	0.0980	10	0.0989
11	0.0998	12	0.1009	13	0.1022	14	0.1035	15	0.1060

*** ELEMENTAL DARCY VELOCITY ***

ELEMENT	VELOCITY	ELEMENT	VELOCITY	ELEMENT	VELOCITY	ELEMENT	VELOCITY
1	12.4	2	12.2	3	12.1	4	12.0
5	11.9	6	11.7	7	11.7	8	11.6
9	11.6	10	11.5	11	11.5	12	11.5
13	11.5	14	11.5	15	11.5		

****
*** ELAPSED SIMULATION TIME : 1.500 ***
****

CUMULATIVE NUMBER OF COMPUTATIONAL TIME STEPS : 3

CURRENT VALUE OF COMPUTATIONAL TIME STEP (DT) : 0.50000E+00

* NODAL PRESSURE VALUES *

NODE	PRESSURE	NODE	PRESSURE	NODE	PRESSURE	NODE	PRESSURE	NODE	PRESSURE
1	-110.6	2	-113.5	3	-116.4	4	-116.7	5	-116.9
6	-117.2	7	-117.4	8	-117.7	9	-118.0	10	-115.9
11	-113.6	12	-111.2	13	-108.7	14	-106.0	15	-103.1
16	-100.0								

*** VOLUMETRIC FLOW BALANCE INFORMATION AT TIME = 0.1500E+01***

SUMMARY OF FLOW MASS BALANCE

```
FLUID FLUX VALUE AT FIRST NODE      =  0.1125E+02
FLUID FLUX VALUE AT LAST NODE       = -0.1134E+02
NET VALUE OF FLUID FLUX             = -0.8237E-01
NET RATE OF VOLUMETRIC STORAGE      = -0.8554E-01
FLOW BALANCE ERROR                  =  0.3171E-02
CUMULATIVE VOLUMETRIC STORAGE       = -0.6370E+00
CUMULATIVE INFLOW VOLUME            =  0.1500E+02
CUMULATIVE OUTFLOW VOLUME           = -0.1564E+02
```

*** LIST OF PARTIALLY SATURATED ELEMENTS ***

ELEM.	SAT. VALUE	ELEM.	SAT. VALUE	ELEM.	SAT. VALUE	ELEM.	SAT. VALUE	ELEM.	SAT. VALUE
1	0.6853	2	0.6804	3	0.4759	4	0.4755	5	0.4750
6	0.4746	7	0.4741	8	0.4737	9	0.0978	10	0.0987
11	0.0997	12	0.1008	13	0.1021	14	0.1035	15	0.1060

*** ELEMENTAL DARCY VELOCITY ***

ELEMENT	VELOCITY	ELEMENT	VELOCITY	ELEMENT	VELOCITY	ELEMENT	VELOCITY
1	11.3	2	11.3	3	11.3	4	11.3
5	11.3	6	11.3	7	11.3	8	11.3
9	11.3	10	11.3	11	11.3	12	11.3
13	11.3	14	11.3	15	11.3		

```
**********************************************
*** ELAPSED SIMULATION TIME :    2.000     ***
**********************************************

     CUMULATIVE NUMBER OF COMPUTATIONAL TIME STEPS :       4

     CURRENT VALUE OF COMPUTATIONAL TIME STEP (DT) :      0.50000E+00
```

* NODAL PRESSURE VALUES *

NODE	PRESSURE	NODE	PRESSURE	NODE	PRESSURE	NODE	PRESSURE	NODE	PRESSURE
1	-117.8	2	-119.9	3	-122.2	4	-122.0	5	-121.8
6	-121.6	7	-121.4	8	-121.3	9	-121.1	10	-118.6
11	-116.0	12	-113.1	13	-110.1	14	-106.9	15	-103.6
16	-100.0								

```
     *** VOLUMETRIC FLOW BALANCE INFORMATION AT TIME =   0.2000E+01***
```

SUMMARY OF FLOW MASS BALANCE

FLUID FLUX VALUE AT FIRST NODE = 0.1001E+02
FLUID FLUX VALUE AT LAST NODE = -0.1032E+02
NET VALUE OF FLUID FLUX = -0.3131E+00
NET RATE OF VOLUMETRIC STORAGE = -0.3258E+00
FLOW BALANCE ERROR = 0.1261E-01
CUMULATIVE VOLUMETRIC STORAGE = -0.7999E+00
CUMULATIVE INFLOW VOLUME = 0.2001E+02
CUMULATIVE OUTFLOW VOLUME = -0.2080E+02

*** LIST OF PARTIALLY SATURATED ELEMENTS ***

ELEM.	SAT. VALUE	ELEM.	SAT. VALUE	ELEM.	SAT. VALUE	ELEM.	SAT. VALUE	ELEM.	SAT. VALUE
1	0.6739	2	0.6705	3	0.4666	4	0.4669	5	0.4672
6	0.4675	7	0.4678	8	0.4680	9	0.0966	10	0.0977
11	0.0988	12	0.1001	13	0.1015	14	0.1031	15	0.1060

*** ELEMENTAL DARCY VELOCITY ***

ELEMENT	VELOCITY	ELEMENT	VELOCITY	ELEMENT	VELOCITY	ELEMENT	VELOCITY
1	10.0	2	10.1	3	10.1	4	10.2
5	10.2	6	10.2	7	10.3	8	10.3
9	10.3	10	10.3	11	10.3	12	10.3
13	10.3	14	10.3	15	10.3		

****
*** ELAPSED SIMULATION TIME : 2.500 ***
****

CUMULATIVE NUMBER OF COMPUTATIONAL TIME STEPS : 5

CURRENT VALUE OF COMPUTATIONAL TIME STEP (DT) : 0.50000E+00

* NODAL PRESSURE VALUES *

NODE	PRESSURE	NODE	PRESSURE	NODE	PRESSURE	NODE	PRESSURE	NODE	PRESSURE
1	-149.4	2	-148.4	3	-147.4	4	-145.2	5	-143.1
6	-141.1	7	-139.0	8	-137.1	9	-135.1	10	-130.6
11	-125.9	12	-121.0	13	-116.0	14	-110.9	15	-105.5

16 -100.0

*** VOLUMETRIC FLOW BALANCE INFORMATION AT TIME = 0.2500E+01***

SUMMARY OF FLOW MASS BALANCE

FLUID FLUX VALUE AT FIRST NODE = 0.5007E+01
FLUID FLUX VALUE AT LAST NODE = -0.6215E+01
NET VALUE OF FLUID FLUX = -0.1209E+01
NET RATE OF VOLUMETRIC STORAGE = -0.1222E+01
FLOW BALANCE ERROR = 0.1297E-01
CUMULATIVE VOLUMETRIC STORAGE = -0.1411E+01
CUMULATIVE INFLOW VOLUME = 0.2251E+02
CUMULATIVE OUTFLOW VOLUME = -0.2390E+02

*** LIST OF PARTIALLY SATURATED ELEMENTS ***

ELEM.	SAT. VALUE	ELEM.	SAT. VALUE	ELEM.	SAT. VALUE	ELEM.	SAT. VALUE	ELEM.	SAT. VALUE
1	0.6308	2	0.6321	3	0.4319	4	0.4346	5	0.4373
6	0.4401	7	0.4428	8	0.4455	9	0.0922	10	0.0937
11	0.0953	12	0.0972	13	0.0993	14	0.1017	15	0.1060

*** ELEMENTAL DARCY VELOCITY ***

ELEMENT	VELOCITY	ELEMENT	VELOCITY	ELEMENT	VELOCITY	ELEMENT	VELOCITY
1	5.11	2	5.29	3	5.45	4	5.59
5	5.72	6	5.85	7	5.96	8	6.06
9	6.09	10	6.11	11	6.13	12	6.15
13	6.17	14	6.19	15	6.22		

***** SAMFT1D HAS SOLVED THE PROBLEM *****

****
*** CPU TIME USED: 8.901 SECS. ***
****

3) Summary of geometry of the problem and material properties;

4) Summary of prescribed boundary conditions and initial nodal values of the primary variable;

5) For each selected output time value:

- nodal values of pressure head
- summary of the flow mass balance
- element values of saturation
- element values of Darcy velocity.

6) CPU time for the simulation. Note that the printed value corresponds to execution on a 25 MHz 80386 computer.

10.4 SINGLE PHASE TRANSPORT SIMULATION PROBLEM

10.4.1 Input Data

The input data file for the sample single-phase transport simulation problem is shown in Table 10.4.1. This problem corresponds to the example flow problem of Section 10.3. The domain geometry and time stepping parameters are the same as those for the flow problem (Table 10.3.1). The velocity and saturation output from the flow simulation are used to define advection and dispersion for the transport simulation. The information is read from an external binary file, by setting parameter NVREAD=1 (group 5). The soil is taken to be initially solute-free; i.e., the initial condition (group 8) is set to zero. The solute is present at the soil surface with a unit relative concentration. No boundary condition is specified for the lower boundary. The numerical solution at the bottom of the soil profile will therefore default to a zero concentration gradient condition.

Table 10.4.1 Input Data for the Single-Phase Transport Simulation Problem.

```
  1    1                                                                  GROUP 1
SAMFT1D SINGLE PHASE MODULE: TRANSPORT IN ROOTZONE  (VAM2D 4.3.5)          ...2
  0    2    1    0    1    0    1    5   15    3    0                     ...3
  1   10    0        0.0        0.0        1.0        0.0        0.0      ...4
  1    0    0    0    0    1    1    1    0    0    0    0    0    0      ...5
     0.0        0.5        0.1        0.5   1.00E09                       .6A1
     0.0                                                                  ...8
     2.0        1.0        1.0        0.41       1.65                     .10A
     2.0        1.0        1.0        0.43       1.55                     ....
     2.0        1.0        1.0        0.45       1.50                     ....
     0.0        0.0                                                       .10B
     0.0        0.0                                                       .10C
     0.0        0.0                                                       ....
     0.0        0.0                                                       ....
  3    0        1.0    0                                                 ..11
  1    2    3        10.0                                                ..12
  2    6    2        30.0                                                ....
  3    7    1        60.0                                                ....
  1    0    0    0                                                       ..13
  1    1        1.0                                                       .14A
  0        0.0                                                           ..18
  1        1.0        0.0                                                ..19
```

10.4.2 Output

Output for the transport simulation problem is listed in Table 10.4.2. The output file is organized as follows:

1) Summary of input control parameters;

2) List of generated simulation time values;

3) Summary of the problem geometry and material properties;

4) Summary of prescribed boundary conditions and the initial nodal concentration values;

5) For each selected output time value:

   - nodal values of concentration
   - element values of saturation
   - element values of Darcy velocity.

   The saturation and velocity values are obtained from the flow simulation; their values are printed here to enable verification that they are identical to the flow simulation results shown in Table 10.3.2.

6) CPU time for the simulation (for 80386 computer).

Table 10.4.2 Output for the Single-Phase Transport Simulation Problem.

```
PROBLEM IDENTIFICATION NUMBER =    1


PROBLEM TITLE
-------------------------------------------------------------------------------

 SAMFT1D SINGLE PHASE MODULE: TRANSPORT IN ROOTZONE  (VAM2D 4.3.5)

-------------------------------------------------------------------------------


PROBLEM SPECIFICATION PARAMETERS
--------------------------------
MODEL OPTION PARAMETER ....................(IMODL) =    0
  NOTE:  IMODL = 0 FOR SOLUTE TRANSPORT ONLY
               = 1 FOR FLUID FLOW ONLY
               = 2 FOR COUPLED FLOW AND TRANSPORT
TOTAL NUMBER OF FLUID PHASES.............. (NTPHAS) =    2
NUMBER OF ACTIVE FLUID PHASES............. (NMPHAS) =    1
HYSTERESIS CONSIDERATION (1=YES,0=NO).....(IHYST) =    0
TOTAL NUMBER OF PRIMARY DEPENDENT VARIABLES(NVAR) =    1
STEADY STATE SIMULATION(1=YES, 0=NO)......(ISSTA) =    0
TIME STEP GENERATION INDEX (1=YES, 0=NO) .(ITSGN) =    1
NUMBER OF TIME STEPS ......................(NTS) =    5
TOTAL NUMBER OF ELEMENTS ..................(NE) =   15
NUMBER OF POROUS MATERIALS .................(NMAT) =    3
SOIL CONSTITUTIVE DATA(0=FUNCTION,1=TABLE)(KPROP) =    0
INITIAL CONDITION NON-UNIFORMITY INDEX ....(NONU) =    0


INPUT / OUTPUT CONTROL PARAMETERS
---------------------------------
VELOCITY/INPUT.............................(NVREAD) =    1
BOUNDARY NODE DATA READ (1=YES, 0=NO)....(IOUTLT) =    0
NUMBER OF NODES FOR WHICH I.C. ARE READ....(NPIN) =    0
OUTPUT REQUIREMENT INDICATOR:
 (0=ALL DATA, 1=NO ELEMENT DATA,
  2=NO DATA, 3=NO MESH AND I.C. DATA.......(IPRD) =    0
UNIT 9 OUTPUT OF VEL / SAT (1=YES, 0=NO).(NVWRIT) =    0
VELOCITY PRINTOUT CONTROL INDEX............(NVPR) =    1
UNIT 10 AND/OR 11 FOR PLOT (0=NO,>0=YES)..(NPLOT) =    1
TIME STEP INCREMENT FOR OUTPUT PRINT OUT..(NSTEP) =    1
OBSERVATION NODE INDEX.....................(IOBSND) =    0
MASS BALANCE TO BE PERFORMED (1=YES,0=NO).(IMBAL) =    0
UNIT 8 OUTPUT OF HEAD/CONC (1=YES, 0=NO).(NOWRIT) =    0
PRINT CHECK OPTION INDEX.................(IPRCHK) =    0
NO. OF SPECIFIED T VALUES FOR PRINTOUT...(NPCORN) =    0

TIME STEP. PARAMETER FOR TRANSPORT SIMULATION.(IKALL) =    1


TEMPORAL DISCRETIZATION DATA
----------------------------
INITIAL TIME VALUE ......................... (TIMA) =  0.0000E+00
VALUE OF FIRST TIME STEP ................... (TIN) =  0.5000E+00
MINIMUM TIME STEP SIZE...................... (TMIN) =  0.1000E+00
MAXIMUM TIME STEP SIZE ..................... (TMAX) =  0.5000E+00
FINAL TIME VALUE OF THE SIMULATION......... (TEND) =  0.1000E+10


DEFAULT INITIAL CONDITION FOR TRANSPORT PROBLEM
-----------------------------------------------
PRESCRIBED INITIAL CONCENTRATION VALUE....(CIDFAL) =  0.0000E+00
```

```
TRANSPORT PROPERTIES OF POROUS MEDIA
------------------------------------


MATERIAL NUMBER (I):    1

LONGITUDINAL DISPERSIVITY.............(PROPJ(I,1)) =  0.2000E+01
TORTUOSITY FACTOR..................  ..(PROPJ(I,2)) =  0.1000E+01
EXPONENT OF MOL. DIFF. COEFF..........(PROPJ(I,3)) =  0.1000E+01
EFFECTIVE POROSITY(0 FOR STEADY STATE)(PROPJ(I,4)) =  0.4100E+00
BULK DENSITY..........................(PROPJ(I,5)) =  0.1650E+01

MATERIAL NUMBER (I):    2

LONGITUDINAL DISPERSIVITY.............(PROPJ(I,1)) =  0.2000E+01
TORTUOSITY FACTOR..................  ..(PROPJ(I,2)) =  0.1000E+01
EXPONENT OF MOL. DIFF. COEFF..........(PROPJ(I,3)) =  0.1000E+01
EFFECTIVE POROSITY(0 FOR STEADY STATE)(PROPJ(I,4)) =  0.4300E+00
BULK DENSITY..........................(PROPJ(I,5)) =  0.1550E+01

MATERIAL NUMBER (I):    3

LONGITUDINAL DISPERSIVITY.............(PROPJ(I,1)) =  0.2000E+01
TORTUOSITY FACTOR..................  ..(PROPJ(I,2)) =  0.1000E+01
EXPONENT OF MOL. DIFF. COEFF..........(PROPJ(I,3)) =  0.1000E+01
EFFECTIVE POROSITY(0 FOR STEADY STATE)(PROPJ(I,4)) =  0.4500E+00
BULK DENSITY..........................(PROPJ(I,5)) =  0.1500E+01

MOLECULAR DIFFUSION COEFFICIENT OF PHASE 1 THROUGH NTPHAS
---------------------------------------------------------

      0.000E+00      0.000E+00


SOLUTE PROPERTIES
-----------------

MATERIAL NUMBER (I) :    1
---------------------
DECAY COEFFICIENT ..................... (RPROP(I,1)) =  0.0000E+00
DISTRIBUTION COEF. FOR PH.#1 & SOIL.. (RPROP(I,2)) =  0.0000E+00

MATERIAL NUMBER (I) :    2
---------------------
DECAY COEFFICIENT ..................... (RPROP(I,1)) =  0.0000E+00
DISTRIBUTION COEF. FOR PH.#1 & SOIL.. (RPROP(I,2)) =  0.0000E+00

MATERIAL NUMBER (I) :    3
---------------------
DECAY COEFFICIENT ..................... (RPROP(I,1)) =  0.0000E+00
DISTRIBUTION COEF. FOR PH.#1 & SOIL.. (RPROP(I,2)) =  0.0000E+00


GRID GENERATION PARAMETERS
--------------------------
NUMBER OF SOIL LAYERS.....................(NLAYER) =    3
PARAMETER INDICATING THE GRID TYPE (IBCGR)
(0=MESH-CENTERED (F.E.), 1=BLOCK-CENTERED(F.D.))...=    0
PARAMETER INDICATING GRID ORIENTATION.....(IHORGR) =    0
IHORGR=0 FOR VERTICAL FLOW, IHORGR=1 FOR HORIZONTAL FLOW



LAYERED GRID DATA
-----------------

LAYER NUMBER :    1
------------------
```

```
NO. OF ELEMENTS (OR GRID BLOCKS) .....(NELM) =    2
MATERIAL NUMBER .....(IMATL) =    3
LAYER THICKNESS.....(THL) =  0.1000E+02

LAYER NUMBER :    2
------------------
NO. OF ELEMENTS (OR GRID BLOCKS) .....(NELM) =    6
MATERIAL NUMBER .....(IMATL) =    2
LAYER THICKNESS.....(THL) =  0.3000E+02

LAYER NUMBER :    3
------------------
NO. OF ELEMENTS (OR GRID BLOCKS) .....(NELM) =    7
MATERIAL NUMBER .....(IMATL) =    1
LAYER THICKNESS.....(THL) =  0.6000E+02


************************************************
*** MESH-CENTERED FINITE ELEMENT GRID IS USED ***
************************************************
```

NODE	Z-COOR.	NODE	Z-COOR.	NODE	Z-COOR.	NODE	Z-COOR.
1	0.00	2	5.00	3	10.00	4	15.00
5	20.00	6	25.00	7	30.00	8	35.00
9	40.00	10	48.57	11	57.14	12	65.71
13	74.29	14	82.86	15	91.43	16	100.00

ELEMENT	MATL. NO.	ELEMENT	MATL. NO.	ELEMENT	MATL. NO.	ELEMENT	MATL. NO.
1	3	2	3	3	2	4	2
5	2	6	2	7	2	8	2
9	1	10	1	11	1	12	1
13	1	14	1	15	1		

```
BOUNDARY CONDITION DATA
-----------------------

NO. OF STEADY DIRICHLET BOUNDARY CONDITIONS....(NBTO) =    1
NO. OF STEADY FLUX BOUNDARY CONDITIONS..... (NDFLUX) =    0
NO. OF TRANSIENT DIRICHLET BOUNDARY CONDITIONS(NBHVAR)=    0
NO. OF TRANSIENT FLUX BOUNDARY CONDITIONS... (NBFVAR) =    0


STEADY-STATE DIRICHLET BOUNDARY CONDITIONS
------------------------------------------

INDEX  NODE NO.     MDEGB(I)     PRESCRIBED VALUE
-----  -----------  -----------  ----------------

   1         1          1            1.000


*** DEFAULT INITIAL CONDITION ***
---------------------------------


INITIAL VALUES OF DEPENDENT VARIABLE #   1
-----------------------------------------
```

NODE NUMBER	DEPENDENT VARIABLE	NODE NUMBER	DEPENDENT VARIABLE	NODE NUMBER	DEPENDENT VARIABLE	NODE NUMBER	DEPENDENT VARIABLE	NODE NUMBER	DEPENDENT VARIABLE

1	0.0000E+00	2	0.0000E+00	3	0.0000E+00	4	0.0000E+00	5	0.0000E+00
6	0.0000E+00	7	0.0000E+00	8	0.0000E+00	9	0.0000E+00	10	0.0000E+00
11	0.0000E+00	12	0.0000E+00	13	0.0000E+00	14	0.0000E+00	15	0.0000E+00
16	0.0000E+00								

TRANSPORT SIMULATION CONTROL DATA

STEADY-STATE VELOCITY FIELD (0=NO,1=YES)..(IVSTED) = 0
UPSTREAM FACTOR .....(WFAC) = 0.00E+00

DEFAULT PHASE SATURATION AND DARCY VELOCITY VALUES

FLUID PHASE NUMBER 1

PHASE SATURATION (DEFAULT VALUE)..... = 0.1000E+01
DEFAULT VALUE OF DARCY VELOCITY ..... = 0.0000E+00

****
*** ELAPSED SIMULATION TIME : 0.5000 ***
****

CUMULATIVE NUMBER OF COMPUTATIONAL TIME STEPS : 1

CURRENT VALUE OF COMPUTATIONAL TIME STEP (DT) : 0.50000E+00

*** NODAL CONCENTRATION VALUES ***

NODE	CONC. VALUE	NODE	CONC. VALUE	NODE	CONC. VALUE	NODE	CONC. VALUE	NODE	CONC. VALUE
1	1.000	2	0.7319	3	0.5229	4	0.4058	5	0.3172
6	0.2495	7	0.1976	8	0.1560	9	0.1341	10	0.1238
11	0.1142	12	0.1054	13	9.6995E-02	14	8.9569E-02	15	8.1570E-02
16	7.6859E-02								

*** LIST OF PARTIALLY SATURATED ELEMENTS ***

ELEM.	SAT. VALUE	ELEM.	SAT. VALUE	ELEM.	SAT. VALUE	ELEM.	SAT. VALUE	ELEM.	SAT. VALUE
1	0.6488	2	0.6490	3	0.4477	4	0.4498	5	0.4518
6	0.4538	7	0.4556	8	0.4572	9	0.0945	10	0.0958
11	0.0972	12	0.0987	13	0.1005	14	0.1025	15	0.1060

*** ELEMENTAL DARCY VELOCITY ***

ELEMENT	VELOCITY	ELEMENT	VELOCITY	ELEMENT	VELOCITY	ELEMENT	VELOCITY
1	6.38	2	6.65	3	6.91	4	7.17
5	7.41	6	7.65	7	7.87	8	8.09
9	8.17	10	8.25	11	8.31	12	8.37
13	8.41	14	8.44	15	8.45		

```
***********************************************
*** ELAPSED SIMULATION TIME :    1.000     ***
***********************************************

   CUMULATIVE NUMBER OF COMPUTATIONAL TIME STEPS :       2

   CURRENT VALUE OF COMPUTATIONAL TIME STEP (DT) :      0.50000E+00

         *** NODAL CONCENTRATION VALUES ***
         -------------------------
```

NODE	CONC. VALUE	NODE	CONC. VALUE	NODE	CONC. VALUE	NODE	CONC. VALUE	NODE	CONC. VALUE
1	1.000	2	0.9509	3	0.8800	4	0.8122	5	0.7402
6	0.6679	7	0.5983	8	0.5298	9	0.4889	10	0.4682
11	0.4478	12	0.4280	13	0.4083	14	0.3900	15	0.3693
16	0.3568								

```
         *** LIST OF PARTIALLY SATURATED ELEMENTS ***
         -------------------------------------------
```

ELEM.	SAT. VALUE	ELEM.	SAT. VALUE	ELEM.	SAT. VALUE	ELEM.	SAT. VALUE	ELEM.	SAT. VALUE
1	0.6900	2	0.6839	3	0.4787	4	0.4777	5	0.4768
6	0.4760	7	0.4753	8	0.4746	9	0.0980	10	0.0989
11	0.0998	12	0.1009	13	0.1022	14	0.1035	15	0.1060

```
         *** ELEMENTAL DARCY VELOCITY ***
         -------------------------------
```

ELEMENT	VELOCITY	ELEMENT	VELOCITY	ELEMENT	VELOCITY	ELEMENT	VELOCITY
1	12.4	2	12.2	3	12.1	4	12.0
5	11.9	6	11.7	7	11.7	8	11.6
9	11.6	10	11.5	11	11.5	12	11.5
13	11.5	14	11.5	15	11.5		

```
***********************************************
*** ELAPSED SIMULATION TIME :    1.500     ***
***********************************************

   CUMULATIVE NUMBER OF COMPUTATIONAL TIME STEPS :       3

   CURRENT VALUE OF COMPUTATIONAL TIME STEP (DT) :      0.50000E+00

         *** NODAL CONCENTRATION VALUES ***
         -------------------------
```

NODE	CONC. VALUE	NODE	CONC. VALUE	NODE	CONC. VALUE	NODE	CONC. VALUE	NODE	CONC. VALUE
1	1.000	2	0.9897	3	0.9707	4	0.9471	5	0.9161
6	0.8788	7	0.8366	8	0.7886	9	0.7579	10	0.7414
11	0.7244	12	0.7073	13	0.6894	14	0.6723	15	0.6519
16	0.6392								

*** LIST OF PARTIALLY SATURATED ELEMENTS ***

ELEM.	SAT. VALUE	ELEM.	SAT. VALUE	ELEM.	SAT. VALUE	ELEM.	SAT. VALUE	ELEM.	SAT. VALUE
1	0.6853	2	0.6804	3	0.4759	4	0.4755	5	0.4750
6	0.4746	7	0.4741	8	0.4737	9	0.0978	10	0.0987
11	0.0997	12	0.1008	13	0.1021	14	0.1035	15	0.1060

*** ELEMENTAL DARCY VELOCITY ***

ELEMENT	VELOCITY	ELEMENT	VELOCITY	ELEMENT	VELOCITY	ELEMENT	VELOCITY
1	11.3	2	11.3	3	11.3	4	11.3
5	11.3	6	11.3	7	11.3	8	11.3
9	11.3	10	11.3	11	11.3	12	11.3
13	11.3	14	11.3	15	11.3		

****
*** ELAPSED SIMULATION TIME : 2.000 ***
****

CUMULATIVE NUMBER OF COMPUTATIONAL TIME STEPS : 4

CURRENT VALUE OF COMPUTATIONAL TIME STEP (DT) : 0.50000E+00

*** NODAL CONCENTRATION VALUES ***

NODE	CONC. VALUE	NODE	CONC. VALUE	NODE	CONC. VALUE	NODE	CONC. VALUE	NODE	CONC. VALUE
1	1.000	2	0.9976	3	0.9925	4	0.9852	5	0.9741
6	0.9588	7	0.9392	8	0.9140	9	0.8970	10	0.8875
11	0.8774	12	0.8668	13	0.8553	14	0.8440	15	0.8300
16	0.8211								

*** LIST OF PARTIALLY SATURATED ELEMENTS ***

ELEM.	SAT. VALUE	ELEM.	SAT. VALUE	ELEM.	SAT. VALUE	ELEM.	SAT. VALUE	ELEM.	SAT. VALUE
1	0.6739	2	0.6705	3	0.4666	4	0.4669	5	0.4672
6	0.4675	7	0.4678	8	0.4680	9	0.0966	10	0.0977
11	0.0988	12	0.1001	13	0.1015	14	0.1031	15	0.1060

*** ELEMENTAL DARCY VELOCITY ***

ELEMENT	VELOCITY	ELEMENT	VELOCITY	ELEMENT	VELOCITY	ELEMENT	VELOCITY

1	10.0	2	10.1	3	10.1	4	10.2
5	10.2	6	10.2	7	10.3	8	10.3
9	10.3	10	10.3	11	10.3	12	10.3
13	10.3	14	10.3	15	10.3		

****
*** ELAPSED SIMULATION TIME : 2.500 ***
****

CUMULATIVE NUMBER OF COMPUTATIONAL TIME STEPS : 5

CURRENT VALUE OF COMPUTATIONAL TIME STEP (DT) : 0.50000E+00

*** NODAL CONCENTRATION VALUES ***

NODE	CONC. VALUE	NODE	CONC. VALUE	NODE	CONC. VALUE	NODE	CONC. VALUE	NODE	CONC. VALUE
1	1.000	2	0.9991	3	0.9972	4	0.9942	5	0.9893
6	0.9819	7	0.9717	8	0.9575	9	0.9477	10	0.9420
11	0.9357	12	0.9291	13	0.9216	14	0.9142	15	0.9045
16	0.8983								

*** LIST OF PARTIALLY SATURATED ELEMENTS ***

ELEM.	SAT. VALUE	ELEM.	SAT. VALUE	ELEM.	SAT. VALUE	ELEM.	SAT. VALUE	ELEM.	SAT. VALUE
1	0.6308	2	0.6321	3	0.4319	4	0.4346	5	0.4373
6	0.4401	7	0.4428	8	0.4455	9	0.0922	10	0.0937
11	0.0953	12	0.0972	13	0.0993	14	0.1017	15	0.1060

*** ELEMENTAL DARCY VELOCITY ***

ELEMENT	VELOCITY	ELEMENT	VELOCITY	ELEMENT	VELOCITY	ELEMENT	VELOCITY
1	5.11	2	5.29	3	5.45	4	5.59
5	5.72	6	5.85	7	5.96	8	6.06
9	6.09	10	6.11	11	6.13	12	6.15
13	6.17	14	6.19	15	6.22		

***** SAMFT1D HAS SOLVED THE PROBLEM *****

****
*** CPU TIME USED: 19.18 SECS. ***
****

10.5 THREE-PHASE FLOW SIMULATION PROBLEM

10.5.1 Input Data

Input data for this sample three-phase flow problem is presented in Table 10.5.1 (See Section 4.4.7 for problem prescription). Note that the automatic block-centered mesh generation option is used by setting IBCGR equal to 1. Because the output control parameter IPRD is set equal to 0, the mesh data and initial condition data will appear in the printed output. All the relative permeability and capillary pressure data are input in a tabulated form in Group 9D. Finally, the boundary condition data shown in Table 10.5.1 contains two injection flux conditions for the two liquid phase.

Table 10.5.1 Input Data for the Three-Phase Flow Simulation Problem

```
   1    1                                                                    GROUP 1
   TEST OF SAMFT1D MODULE FOR THREE-PHASE FLOW                               GROUP 2
   1    3    3    0    3    0    1   40   20    1    1    2                 GROUP 3
   1   10    1        .01     1.0E5 9.8066E00 1.00000E5      .001    0.001 GROUP 4
   0    0    1    0    0    0    0   10    0    1    0    0    5            GROUP 5
      0.0   1.00E04       100.  8.6400E6   1.00E20                         GROUP 6A
   3    2       0.0 1.00000E5       10.0                                    GROUP 7A
   1    1      .250   0.300E0                                               GROUP 7B
   2    1      10.0   1.000E0                                               GROUP 7B
1.000E-12    1.E-10       0.3       0.2       0.10                         GROUP 9A
    1.E03   1.00E-3    4.3E-9                                               GROUP 9B
  9.50E02   1.00E-3    3.0E-9                                               GROUP 9B
1.1774E00 1.983E-5 1.1774E-5                                               GROUP 9B
   9    9       0.2       0.0        .68                                   GROUP 9D
.2000E00  .0000E00  .6800E00  0.9000E04                                    GROUP 9D
.3000E00  .0400E00  .5500E00  0.5400E04                                    GROUP 9D
.4000E00  .1000E00  .4300E00  0.3900E04                                    GROUP 9D
.5000E00  .1800E00  .3100E00  0.3300E04                                    GROUP 9D
.6000E00  .3000E00  .2000E00  0.3000E04                                    GROUP 9D
.7000E00  .4400E00  .1200E00  0.2700E04                                    GROUP 9D
.8000E00  .6000E00  .0500E00  0.2400E04                                    GROUP 9D
.9000E00  .8000E00  .0000E00  0.1530E04                                    GROUP 9D
1.000E00  1.000E00  .0000E00  0.0000E00                                    GROUP 9D
 .000E00   .000E00  .6800E00  0.0000E00 0.0000E00                          GROUP 9D
 .100E00   .010E00  .4900E00  0.9000E03 1.0000E03                          GROUP 9D
 .200E00   .040E00  .3400E00  1.2000E03 2.0000E03                          GROUP 9D
 .300E00   .090E00  .2100E00  1.5000E03 3.0000E03                          GROUP 9D
 .400E00   .160E00  .1160E00  1.8000E03 3.3000E03                          GROUP 9D
 .500E00   .250E00  .0450E00  2.1000E03 3.6000E03                          GROUP 9D
 .600E00   .360E00  .0009E00  2.4000E03 3.9000E03                          GROUP 9D
 .680E00   .460E00  .0000E00  3.0000E03 4.5000E03                          GROUP 9D
 .800E00   .640E00  .0000E00  9.0000E03 6.6000E03                          GROUP 9D
   1    1      1.E0    0                                                   GROUP 11
   1   20    1      10.0                                                   GROUP 12
   1    1    0    1    3    2                                              GROUP 13
  20    0 1.0000E05                                                        GROUP 14A
   1    1 3.1709E-6                                                        GROUP 14B
   1    2    2    1                                                        GROUP 16A
  .648E07  2.000E10                                                        GROUP 16B
2.8538E-5  0.000E00                                                        GROUP 16C
8.6400E05 6.4800E06 8.6400E06 4.3200E07 8.6400E07                          GROUP 22
```

10.5.2 Output

The output from the line printer for this three-phase flow problem is displayed in Table 10.5.2. This output, which corresponds to input data in Table 10.5.1, consists of the following categories of information:

1. Brief summary of control input data and material properties.
2. Relative permeability and capillary pressure data.
3. Mesh data.
4. Prescribed boundary condition data.
5. Element numbers, centroidal coordinates and discretization.
6. Time-step number and time value.
7. Convergence summary of the nonlinear iterations.
8. Node numbers and nodal pressure and saturation values corresponding to the given time value for the three phases.
9. Mass balance budget.

Note that information in categories 6 through 9 are repeated for each time step.

Table 10.5.2. Output for the Three-Phase Flow Simulation Problem.

```
PROBLEM IDENTIFICATION NUMBER =    1

PROBLEM TITLE
-------------------------------------------------------------------------------

    TEST OF SAMFT1D MODULE FOR THREE-PHASE FLOW

-------------------------------------------------------------------------------


 PROBLEM SPECIFICATION PARAMETERS
--------------------------------
MODEL OPTION PARAMETER .....................(IMODL) =    1
  NOTE:  IMODL = 0 FOR SOLUTE TRANSPORT ONLY
               = 1 FOR FLUID FLOW ONLY
               = 2 FOR COUPLED FLOW AND TRANSPORT
TOTAL NUMBER OF FLUID PHASES..... (NTPHAS) =    3
NUMBER OF ACTIVE FLUID PHASES..... (NMPHAS) =    3
HYSTERESIS CONSIDERATION (1=YES,0=NO).....(IHYST) =    0
TOTAL NUMBER OF PRIMARY DEPENDENT VARIABLES(NVAR) =    3
STEADY STATE SIMULATION(1=YES, 0=NO)......(ISSTA) =    0
TIME STEP GENERATION INDEX (1=YES, 0=NO) .(ITSGN) =    1
NUMBER OF TIME STEPS .......................(NTS) =   40
TOTAL NUMBER OF ELEMENTS ....................(NE) =   20
NUMBER OF POROUS MATERIALS .................(NMAT) =    1
SOIL CONSTITUTIVE DATA(0=FUNCTION,1=TABLE)(KPROP) =    1
INITIAL CONDITION NON-UNIFORMITY INDEX ....(NONU) =    2


INPUT / OUTPUT CONTROL PARAMETERS
---------------------------------
VELOCITY/INPUT.............................(NVREAD) =    0
BOUNDARY NODE DATA READ (1=YES, 0=NO)....(IOUTLT) =    0
NUMBER OF NODES FOR WHICH I.C. ARE READ....(NPIN) =    1
OUTPUT REQUIREMENT INDICATOR:
 (0=ALL DATA, 1=NO ELEMENT DATA,
  2=NO DATA, 3=NO MESH AND I.C. DATA.......(IPRD) =    0
UNIT 9 OUTPUT OF VEL / SAT (1=YES, 0=NO).(NVWRIT) =    0
VELOCITY PRINTOUT CONTROL INDEX............(NVPR) =    0
UNIT 10 AND/OR 11 FOR PLOT (0=NO,>0=YES)..(NPLOT) =    0
TIME STEP INCREMENT FOR OUTPUT PRINT OUT..(NSTEP) =   10
OBSERVATION NODE INDEX.....................(IOBSND) =    0
MASS BALANCE TO BE PERFORMED (1=YES,0=NO).(IMBAL) =    1
UNIT 8 OUTPUT OF HEAD/CONC (1=YES, 0=NO).(NOWRIT) =    0
PRINT CHECK OPTION INDEX.................(IPRCHK) =    0
NO. OF SPECIFIED T VALUES FOR PRINTOUT...(NPCORN) =    5

MAX. NUMBER OF NONLINEAR FLOW ITERATIONS.(NITMAX) =   10
CRITERION NO. OF CONVERGENCE TOLERANCE ..(ICONVG) =    1
ICONVG = 1, FOR RELATIVE TOLERANCE,
ICONVG = 2, FOR ABSOLUTE TOLERANCE.
ABSOLUTE PRESSURE TOLERANCE.................(HTOL) =  0.1000E-01
ABSOLUTE SATURATION TOLERANCE...............(STOL) =  0.1000E+06
GRAVITATIONAL ACCELERATION.................(GCONST) =  0.9807E+01
ATMOSPHERE PRESSURE .......................(Patm) =  0.1000E+06
RELATIVE PRESSURE CONVERGENCE TOLERANCE....(RPTOL) =  0.1000E-02
RELATIVE SATURATION TOLERANCE..............(RSTOL) =  0.1000E-02
TEMPORAL DISCRETIZATION DATA
----------------------------
INITIAL TIME VALUE ..................... (TIMA) =  0.0000E+00
VALUE OF FIRST TIME STEP ................... (TIN) =  0.1000E+05
MINIMUM TIME STEP SIZE..................... (TMIN) =  0.1000E+03
```

```
MAXIMUM TIME STEP SIZE ..................... (TMAX) =  0.8640E+07
FINAL TIME VALUE OF THE SIMULATION......... (TEND) =  0.1000E+21


DEFAULT INITIAL CONDITION DATA FOR FLOW PROBLEM
-----------------------------------------------
INITIAL CONDITION IDENTIFIER.............(IDFVAR) =    3
NUMBER OF CONTROL POINTS REQUIRED TO SPECIFY THE
PROFILE OF INITIAL FUNCTION CORRESPONDING TO THE
SPECIFIED VALUE OF IDFVAR................(NCPONT) =    2
DEFAULT VALUE OF INITIAL SATURATION OF THE NON-
AQUEOUS LIQUID PHASE..................... HFDFAL(1) =     0.000
DEFAULT VALUE OF INITIAL PRESSURE OF THE AIR
PHASE.....................................HIDFAL(2) = 0.100E+06
DEPTH FROM TOP SURFACE OF THE GRID
TO WATER TABLE............................HIDFAL(3) =    10.000


VERTCAL PROFILE FOR INITIAL FUNCTION
------------------------------------

 CONTROL POINT #     MATERIAL #     VERT. COOR.      FUNCTION VALUE
                                  ( + DOWNWARD )
 --------------      ----------     -----------      --------------

      1                1             0.2500          0.3000
      2                1              10.00           1.000


HYDRAULIC PROPERTIES OF POROUS MEDIA
------------------------------------


MATERIAL NUMBER (I):    1

INTRINSIC PERMEABILITY .................(PROP(I,3)) =  0.1000E-11
POROUS MATRIX COMPRESSIBILITY ........ (PROP(I,4)) =  0.1000E-09
EFFECTIVE POROSITY..... ..... (PROP(I,5)) =  0.3000E+00
IRREDUCIBLE NAPL SATURATION IN N-W ....(SNIRWN(I)) =  0.2000E+00
THRESHOLD NAPL SATURATION.... ..........(SNSTR(I)) =  0.1000E+00

FLUID PROPERTIES
----------------

FLUID PHASE NUMBER:    1

REFERENCE DENSITY..................................... =  0.1000E+04
REFERENCE DYNAMIC VISCOSITY........................... =  0.1000E-02
COMPRESSIBILITY ...................................... =  0.4300E-08

FLUID PHASE NUMBER:    2

REFERENCE DENSITY..................................... =  0.9500E+03
REFERENCE DYNAMIC VISCOSITY........................... =  0.1000E-02
COMPRESSIBILITY ...................................... =  0.3000E-08

FLUID PHASE NUMBER:    3

REFERENCE DENSITY..................................... =  0.1177E+01
REFERENCE DYNAMIC VISCOSITY........................... =  0.1983E-04
COMPRESSIBILITY ...................................... =  0.1177E-04

MATERIAL NUMBER (I):    1

IRREDUCIBLE WATER SATURATION.. ........(PROP(I,7)) =  0.2000E+00
Pcnw  AT Sw=1 IN W-N PHASE CONDITION...(PCNSW1(I)) =  0.0000E+00
Kr TO NAPL PHASE AT Sw=Swir(I).........(AKSTAR(I)) =  0.6800E+00

TABULATED REL. PERM. AND CAP. PRESSURE DATA FOR SOIL MATERIAL NUMBER :    1
```

```
------------------------------------------------------------------------

NO. OF ROW ENTRIES FOR PHASE 1 VS. 2 RELATIONSHIPS =    9

  SATURATION-PH1     REL. PERM.-PH1     REL. PERM.-PH21   CAP. PRESSURE-PH21

    0.2000E+00         0.0000E+00         0.6800E+00         0.9000E+04
    0.3000E+00         0.4000E-01         0.5500E+00         0.5400E+04
    0.4000E+00         0.1000E+00         0.4300E+00         0.3900E+04
    0.5000E+00         0.1800E+00         0.3100E+00         0.3300E+04
    0.6000E+00         0.3000E+00         0.2000E+00         0.3000E+04
    0.7000E+00         0.4400E+00         0.1200E+00         0.2700E+04
    0.8000E+00         0.6000E+00         0.5000E-01         0.2400E+04
    0.9000E+00         0.8000E+00         0.0000E+00         0.1530E+04
    0.1000E+01         0.1000E+01         0.0000E+00         0.0000E+00

TABULATED REL. PERM. AND CAP. PRESSURE DATA FOR SOIL MATERIAL NUMBER :    1
------------------------------------------------------------------------

NO.OF ROW ENTRIES FOR PHASE 2 VS. 3 RELATIONSHIPS  =     9

  SATURATION-PH3     REL. PERM.-PH3     REL. PERM.-PH23   CAP. PRESSURE-PH32   CAP. PRESSURE-PH31

    0.0000E+00         0.0000E+00         0.6800E+00         0.0000E+00         0.0000E+00
    0.1000E+00         0.1000E-01         0.4900E+00         0.9000E+03         0.1000E+04
    0.2000E+00         0.4000E-01         0.3400E+00         0.1200E+04         0.2000E+04
    0.3000E+00         0.9000E-01         0.2100E+00         0.1500E+04         0.3000E+04
    0.4000E+00         0.1600E+00         0.1160E+00         0.1800E+04         0.3300E+04
    0.5000E+00         0.2500E+00         0.4500E-01         0.2100E+04         0.3600E+04
    0.6000E+00         0.3600E+00         0.9000E-03         0.2400E+04         0.3900E+04
    0.6800E+00         0.4600E+00         0.0000E+00         0.3000E+04         0.4500E+04
    0.8000E+00         0.6400E+00         0.0000E+00         0.9000E+04         0.6600E+04


GRID GENERATION PARAMETERS
--------------------------
NUMBER OF SOIL LAYERS.....................(NLAYER) =    1
PARAMETER INDICATING THE GRID TYPE (IBCGR)
(0=MESH-CENTERED (F.E.), 1=BLOCK-CENTERED(F.D.))...=    1
CROSS-SECTIONAL AREA OF THE SOIL COLUMN....(ACROS) =  0.1000E+01
PARAMETER INDICATING GRID ORIENTATION.....(IHORGR) =    0
IHORGR=0 FOR VERTICAL FLOW, IHORGR=1 FOR HORIZONTAL FLOW


LAYERED GRID DATA
-----------------

LAYER NUMBER :    1
------------------
NO. OF ELEMENTS (OR GRID BLOCKS) ..........(NELM) =   20
MATERIAL NUMBER ...........................(IMATL) =    1
LAYER THICKNESS............................(THL) =  0.1000E+02


*****************************************************
*** BLOCK-CENTERED FINITE DIFFERENCE GRID IS USED ***
*****************************************************

BLOCK    Z-COOR.    BLOCK    Z-COOR.    BLOCK    Z-COOR.    BLOCK    Z-COOR.
-----    -------    -----    -------    -----    -------    -----    -------

 1         0.25       2         0.75       3         1.25       4         1.75
 5         2.25       6         2.75       7         3.25       8         3.75
 9         4.25      10         4.75      11         5.25      12         5.75
13         6.25      14         6.75      15         7.25      16         7.75
17         8.25      18         8.75      19         9.25      20         9.75
```

BLOCK	VOLUME	BLOCK	VOLUME	BLOCK	VOLUME	BLOCK	VOLUME
1	0.50	2	0.50	3	0.50	4	0.50
5	0.50	6	0.50	7	0.50	8	0.50
9	0.50	10	0.50	11	0.50	12	0.50
13	0.50	14	0.50	15	0.50	16	0.50
17	0.50	18	0.50	19	0.50	20	0.50

BLOCK	DELZ	BLOCK	DELZ	BLOCK	DELZ	BLOCK	DELZ
1	0.50	2	0.50	3	0.50	4	0.50
5	0.50	6	0.50	7	0.50	8	0.50
9	0.50	10	0.50	11	0.50	12	0.50
13	0.50	14	0.50	15	0.50	16	0.50
17	0.50	18	0.50	19	0.50	20	0.50

BOUNDARY CONDITION DATA

NO. OF STEADY DIRICHLET BOUNDARY CONDITIONS....(NBTO) = 1
NO. OF STEADY FLUX BOUNDARY CONDITIONS..... (NDFLUX) = 1
NO. OF TRANSIENT DIRICHLET BOUNDARY CONDITIONS(NBHVAR)= 0
NO. OF TRANSIENT FLUX BOUNDARY CONDITIONS... (NBFVAR) = 1
BOUNDARY SPECIFICATION # OF SURFACE NODE.....(NBCND1) = 3
BOUNDARY SPECIFICATION # OF BOTTOM NODE.....(NBCNDN) = 2

STEADY-STATE DIRICHLET BOUNDARY CONDITIONS

INDEX	NODE NO.	MDEGB(I)	PRESCRIBED VALUE
1	20	0	1.0000E+05

STEADY-STATE FLUX BOUNDARY CONDITIONS

INDEX	NODE NO.	MDEGF(I)	FLUID FLUX
1	1	1	3.1709E-06

TRANSIENT FLUX BOUNDARY CONDITIONS

TIME DEPENDENT FLUX B. C. FOR NODE NO. 1 VALUE OF MDEGFT(I) 2

NUMBER OF CONTROL POINTS IN THE TIME GRAPH = 2
TEMPORAL VARIATION (0=CONTINUOUS, 1=STEP) = 1

TIME VERSUS PRESCRIBED FLUID FLUXES

(TIME)	(FLUID FLUXES)
6.4800E+06	2.8538E-05
2.0000E+10	0.0000E+00

LIST OF TIME VALUES FOR PRINTING SIMULATION RESULT

0.86400E+06 0.64800E+07 0.86400E+07 0.43200E+08 0.86400E+08

```
*******************************************
* ELAPSED SIMULATION TIME =     0.8640E+06 *
*******************************************

     CUMULATIVE NUMBER OF COMPUTATIONAL TIME STEPS =    4

     CURRENT VALUE OF COMPUTATIONAL TIME STEP (DT) =    0.5540E+06

     SUMMARY OF NONLINEAR ITERATION USING RELATIVE CONVERGENCE CRITERION
     ------------------------------------------------------------------
```

ITERATION	NUMBER OF NON-CONVERGENT NODAL VALUES	MAXIMUM RELATIVE ERROR	NODAL UNKNOWN NUMBER
1	7	0.110949E+00	2
2	7	0.180845E-01	3
3	2	0.835736E-02	5
4	1	0.269381E-02	1
5	0	0.375931E-03	1

```
**********************
* SIMULATION RESULTS *
**********************
```

NODE	PRES. (PH. 1)	SAT. (PH. 1)	SAT. (PH. 2)	PRES. (PH. 2)	SAT. (PH. 3)	PRES. (PH. 3)
1	0.8877E+05	0.2087E+00	0.1730E+00	0.9746E+05	0.6183E+00	0.1000E+06
2	0.9341E+05	0.2005E+00	-0.1039E-24	0.9341E+05	0.7995E+00	0.1000E+06
3	0.9341E+05	0.2005E+00	-0.2651E-30	0.9341E+05	0.7995E+00	0.1000E+06
4	0.9341E+05	0.2004E+00	-0.1255E-27	0.9341E+05	0.7996E+00	0.1000E+06
5	0.9341E+05	0.2004E+00	-0.9766E-28	0.9341E+05	0.7996E+00	0.1000E+06
6	0.9341E+05	0.2004E+00	-0.7650E-28	0.9341E+05	0.7996E+00	0.1000E+06
7	0.9341E+05	0.2004E+00	-0.5260E-28	0.9341E+05	0.7996E+00	0.1000E+06
8	0.9341E+05	0.2004E+00	-0.3369E-28	0.9341E+05	0.7996E+00	0.1000E+06
9	0.9341E+05	0.2004E+00	-0.2039E-28	0.9341E+05	0.7996E+00	0.1000E+06
10	0.9341E+05	0.2004E+00	-0.1167E-28	0.9341E+05	0.7996E+00	0.1000E+06
11	0.9341E+05	0.2003E+00	-0.4507E-09	0.9341E+05	0.7997E+00	0.1000E+06
12	0.9342E+05	0.2003E+00	-0.4891E-09	0.9342E+05	0.7997E+00	0.1000E+06
13	0.9342E+05	0.2003E+00	-0.4832E-09	0.9342E+05	0.7997E+00	0.1000E+06
14	0.9342E+05	0.2003E+00	-0.4851E-09	0.9342E+05	0.7997E+00	0.1000E+06
15	0.9342E+05	0.2003E+00	0.1908E-08	0.9342E+05	0.7997E+00	0.1000E+06
16	0.9342E+05	0.2003E+00	0.6359E-30	0.9342E+05	0.7997E+00	0.1000E+06
17	0.9342E+05	0.2002E+00	0.6911E-30	0.9342E+05	0.7998E+00	0.1000E+06
18	0.9342E+05	0.2002E+00	0.7120E-30	0.9342E+05	0.7998E+00	0.1000E+06
19	0.9344E+05	0.2010E+00	0.6397E-28	0.9344E+05	0.7990E+00	0.1000E+06
20	0.9755E+05	0.7529E+00	-0.3052E-29	0.9755E+05	0.2471E+00	0.1000E+06

```
     SUMMARY OF MASS BALANCE COMPUTATION FOR FLOW SIMULATION
     -------------------------------------------------------

     WATER
     -----
     (1) CUMULATIVE (INFLOW-OUTFLOW) MASS                        =    0.2363E+01
     (2) CUMULATIVE MASS STORAGE CHANGES                         =    0.2364E+01
     (3) MASS BALANCE ERROR: (1)-(2)                             =   -0.6006E-03
     (4) RELATIVE MASS BALANCE ERROR: ABS(3)/(ABS(1)+ABS(2))     =    0.1271E-03
```

NAPL
----
(1) CUMULATIVE (INFLOW-OUTFLOW) MASS = 0.2466E+02
(2) CUMULATIVE MASS STORAGE CHANGES = 0.2466E+02
(3) MASS BALANCE ERROR: (1)-(2) = 0.5329E-13
(4) RELATIVE MASS BALANCE ERROR: ABS(3)/(ABS(1)+ABS(2)) = 0.1081E-14

TIME STEP NO. 4 HAS BEEN COMPLETED TOTAL ITERATION NUMBER = 13

****
* ELAPSED SIMULATION TIME = 0.4589E+07 *
****

CUMULATIVE NUMBER OF COMPUTATIONAL TIME STEPS = 10

CURRENT VALUE OF COMPUTATIONAL TIME STEP (DT) = 0.2910E+06

SUMMARY OF NONLINEAR ITERATION USING RELATIVE CONVERGENCE CRITERION

ITERATION	NUMBER OF NON-CONVERGENT NODAL VALUES	MAXIMUM RELATIVE ERROR	NODAL UNKNOWN NUMBER
1	4	0.585196E-01	14
2	5	0.872744E-02	15
3	3	0.664859E-02	13
4	0	0.850988E-03	13

****
* SIMULATION RESULTS *
****

NODE	PRES. (PH. 1)	SAT. (PH. 1)	SAT. (PH. 2)	PRES. (PH. 2)	SAT. (PH. 3)	PRES. (PH. 3)
1	0.8865E+05	0.2008E+00	0.2056E+00	0.9762E+05	0.5936E+00	0.1000E+06
2	0.8865E+05	0.2008E+00	0.2056E+00	0.9762E+05	0.5936E+00	0.1000E+06
3	0.8865E+05	0.2008E+00	0.2056E+00	0.9762E+05	0.5936E+00	0.1000E+06
4	0.8864E+05	0.2008E+00	0.2040E+00	0.9761E+05	0.5951E+00	0.1000E+06
5	0.8792E+05	0.2102E+00	0.9823E-01	0.9640E+05	0.6916E+00	0.1000E+06
6	0.9340E+05	0.2001E+00	-0.1869E-24	0.9340E+05	0.7999E+00	0.1000E+06
7	0.9340E+05	0.2002E+00	-0.1507E-24	0.9340E+05	0.7998E+00	0.1000E+06
8	0.9340E+05	0.2003E+00	0.7561E-21	0.9340E+05	0.7997E+00	0.1000E+06
9	0.9341E+05	0.2004E+00	0.4878E-28	0.9341E+05	0.7996E+00	0.1000E+06
10	0.9341E+05	0.2005E+00	-0.1167E-28	0.9341E+05	0.7995E+00	0.1000E+06
11	0.9341E+05	0.2005E+00	-0.4507E-09	0.9341E+05	0.7995E+00	0.1000E+06
12	0.9342E+05	0.2006E+00	-0.4891E-09	0.9342E+05	0.7994E+00	0.1000E+06
13	0.9342E+05	0.2006E+00	-0.4832E-09	0.9342E+05	0.7994E+00	0.1000E+06
14	0.9342E+05	0.2007E+00	-0.4851E-09	0.9342E+05	0.7993E+00	0.1000E+06
15	0.9342E+05	0.2007E+00	0.1908E-08	0.9342E+05	0.7993E+00	0.1000E+06
16	0.9342E+05	0.2007E+00	0.6359E-30	0.9342E+05	0.7993E+00	0.1000E+06
17	0.9343E+05	0.2008E+00	0.6911E-30	0.9343E+05	0.7992E+00	0.1000E+06
18	0.9343E+05	0.2008E+00	0.7120E-30	0.9343E+05	0.7992E+00	0.1000E+06
19	0.9350E+05	0.2048E+00	0.6397E-28	0.9350E+05	0.7952E+00	0.1000E+06
20	0.9755E+05	0.7532E+00	-0.3052E-29	0.9755E+05	0.2468E+00	0.1000E+06

SUMMARY OF MASS BALANCE COMPUTATION FOR FLOW SIMULATION

WATER

(1) CUMULATIVE (INFLOW-OUTFLOW) MASS = 0.3830E+01
(2) CUMULATIVE MASS STORAGE CHANGES = 0.3833E+01
(3) MASS BALANCE ERROR: (1)-(2) = -0.3226E-02
(4) RELATIVE MASS BALANCE ERROR: ABS(3)/(ABS(1)+ABS(2)) = 0.4210E-03

NAPL

(1) CUMULATIVE (INFLOW-OUTFLOW) MASS = 0.1310E+03
(2) CUMULATIVE MASS STORAGE CHANGES = 0.1310E+03
(3) MASS BALANCE ERROR: (1)-(2) = -0.2718E-08
(4) RELATIVE MASS BALANCE ERROR: ABS(3)/(ABS(1)+ABS(2)) = 0.1038E-10

TIME STEP NO. 10 HAS BEEN COMPLETED TOTAL ITERATION NUMBER = 41

* ELAPSED SIMULATION TIME = 0.5992E+07 *

CUMULATIVE NUMBER OF COMPUTATIONAL TIME STEPS = 20

CURRENT VALUE OF COMPUTATIONAL TIME STEP (DT) = 0.2871E+05

SUMMARY OF NONLINEAR ITERATION USING RELATIVE CONVERGENCE CRITERION

ITERATION	NUMBER OF NON-CONVERGENT NODAL VALUES	MAXIMUM RELATIVE ERROR	NODAL UNKNOWN NUMBER
1	1	0.568498E-02	17
2	0	0.898466E-06	16

* SIMULATION RESULTS *

NODE	PRES. (PH. 1)	SAT. (PH. 1)	SAT. (PH. 2)	PRES. (PH. 2)	SAT. (PH. 3)	PRES. (PH. 3)
1	0.8865E+05	0.2008E+00	0.2056E+00	0.9762E+05	0.5936E+00	0.1000E+06
2	0.8865E+05	0.2008E+00	0.2056E+00	0.9762E+05	0.5936E+00	0.1000E+06
3	0.8865E+05	0.2008E+00	0.2056E+00	0.9762E+05	0.5936E+00	0.1000E+06
4	0.8865E+05	0.2008E+00	0.2056E+00	0.9762E+05	0.5936E+00	0.1000E+06
5	0.8865E+05	0.2009E+00	0.2054E+00	0.9762E+05	0.5938E+00	0.1000E+06
6	0.8894E+05	0.2126E+00	0.1721E+00	0.9748E+05	0.6153E+00	0.1000E+06
7	0.9341E+05	0.2010E+00	-0.1507E-24	0.9341E+05	0.7990E+00	0.1000E+06
8	0.9341E+05	0.2009E+00	0.7561E-21	0.9341E+05	0.7991E+00	0.1000E+06
9	0.9341E+05	0.2008E+00	0.4878E-28	0.9341E+05	0.7992E+00	0.1000E+06
10	0.9341E+05	0.2007E+00	-0.1167E-28	0.9341E+05	0.7993E+00	0.1000E+06
11	0.9341E+05	0.2006E+00	-0.4507E-09	0.9341E+05	0.7994E+00	0.1000E+06
12	0.9341E+05	0.2006E+00	-0.4891E-09	0.9341E+05	0.7994E+00	0.1000E+06

13	0.9342E+05	0.2006E+00	-0.4832E-09	0.9342E+05	0.7994E+00	0.1000E+06
14	0.9342E+05	0.2005E+00	-0.4851E-09	0.9342E+05	0.7995E+00	0.1000E+06
15	0.9342E+05	0.2005E+00	0.1908E-08	0.9342E+05	0.7995E+00	0.1000E+06
16	0.9342E+05	0.2005E+00	0.6359E-30	0.9342E+05	0.7995E+00	0.1000E+06
17	0.9342E+05	0.2005E+00	0.6911E-30	0.9342E+05	0.7995E+00	0.1000E+06
18	0.9342E+05	0.2005E+00	0.7120E-30	0.9342E+05	0.7995E+00	0.1000E+06
19	0.9348E+05	0.2036E+00	0.6397E-28	0.9348E+05	0.7964E+00	0.1000E+06
20	0.9755E+05	0.7532E+00	-0.3052E-29	0.9755E+05	0.2468E+00	0.1000E+06

SUMMARY OF MASS BALANCE COMPUTATION FOR FLOW SIMULATION

WATER

(1) CUMULATIVE (INFLOW-OUTFLOW) MASS = 0.4281E+01
(2) CUMULATIVE MASS STORAGE CHANGES = 0.4285E+01
(3) MASS BALANCE ERROR: (1)-(2) = -0.3720E-02
(4) RELATIVE MASS BALANCE ERROR: ABS(3)/(ABS(1)+ABS(2)) = 0.4343E-03

NAPL

(1) CUMULATIVE (INFLOW-OUTFLOW) MASS = 0.1710E+03
(2) CUMULATIVE MASS STORAGE CHANGES = 0.1710E+03
(3) MASS BALANCE ERROR: (1)-(2) = -0.3583E-08
(4) RELATIVE MASS BALANCE ERROR: ABS(3)/(ABS(1)+ABS(2)) = 0.1048E-10

TIME STEP NO. 20 HAS BEEN COMPLETED TOTAL ITERATION NUMBER = 67

****
* ELAPSED SIMULATION TIME = 0.6480E+07 *
****

CUMULATIVE NUMBER OF COMPUTATIONAL TIME STEPS = 24

CURRENT VALUE OF COMPUTATIONAL TIME STEP (DT) = 0.1378E+06

SUMMARY OF NONLINEAR ITERATION USING RELATIVE CONVERGENCE CRITERION

ITERATION	NUMBER OF NON-CONVERGENT NODAL VALUES	MAXIMUM RELATIVE ERROR	NODAL UNKNOWN NUMBER
1	4	0.285554E-01	20
2	1	0.306659E-02	21
3	0	0.120077E-03	19

****
* SIMULATION RESULTS *
****

NODE	PRES. (PH. 1)	SAT. (PH. 1)	SAT. (PH. 2)	PRES. (PH. 2)	SAT. (PH. 3)	PRES. (PH. 3)
1	0.8865E+05	0.2008E+00	0.2056E+00	0.9762E+05	0.5936E+00	0.1000E+06
2	0.8865E+05	0.2008E+00	0.2056E+00	0.9762E+05	0.5936E+00	0.1000E+06
3	0.8865E+05	0.2008E+00	0.2056E+00	0.9762E+05	0.5936E+00	0.1000E+06
4	0.8865E+05	0.2008E+00	0.2056E+00	0.9762E+05	0.5936E+00	0.1000E+06
5	0.8865E+05	0.2008E+00	0.2056E+00	0.9762E+05	0.5935E+00	0.1000E+06
6	0.8866E+05	0.2015E+00	0.2032E+00	0.9761E+05	0.5954E+00	0.1000E+06

7	0.8889E+05	0.2074E+00	0.6638E-01	0.9468E+05	0.7262E+00	0.1000E+06
8	0.9341E+05	0.2008E+00	0.7559E-21	0.9341E+05	0.7992E+00	0.1000E+06
9	0.9341E+05	0.2009E+00	0.7304E-24	0.9341E+05	0.7991E+00	0.1000E+06
10	0.9342E+05	0.2011E+00	-0.1167E-28	0.9342E+05	0.7989E+00	0.1000E+06
11	0.9342E+05	0.2011E+00	-0.4507E-09	0.9342E+05	0.7989E+00	0.1000E+06
12	0.9342E+05	0.2011E+00	-0.4891E-09	0.9342E+05	0.7989E+00	0.1000E+06
13	0.9343E+05	0.2012E+00	-0.4832E-09	0.9343E+05	0.7988E+00	0.1000E+06
14	0.9343E+05	0.2011E+00	-0.4851E-09	0.9343E+05	0.7989E+00	0.1000E+06
15	0.9343E+05	0.2011E+00	0.1908E-08	0.9343E+05	0.7989E+00	0.1000E+06
16	0.9343E+05	0.2011E+00	0.6359E-30	0.9343E+05	0.7989E+00	0.1000E+06
17	0.9343E+05	0.2011E+00	0.6911E-30	0.9343E+05	0.7989E+00	0.1000E+06
18	0.9343E+05	0.2010E+00	0.7120E-30	0.9343E+05	0.7990E+00	0.1000E+06
19	0.9350E+05	0.2048E+00	0.6397E-28	0.9350E+05	0.7952E+00	0.1000E+06
20	0.9755E+05	0.7532E+00	-0.3052E-29	0.9755E+05	0.2468E+00	0.1000E+06

SUMMARY OF MASS BALANCE COMPUTATION FOR FLOW SIMULATION

WATER

(1) CUMULATIVE (INFLOW-OUTFLOW) MASS = 0.4466E+01
(2) CUMULATIVE MASS STORAGE CHANGES = 0.4471E+01
(3) MASS BALANCE ERROR: (1)-(2) = -0.4340E-02
(4) RELATIVE MASS BALANCE ERROR: ABS(3)/(ABS(1)+ABS(2)) = 0.4856E-03

NAPL

(1) CUMULATIVE (INFLOW-OUTFLOW) MASS = 0.1849E+03
(2) CUMULATIVE MASS STORAGE CHANGES = 0.1849E+03
(3) MASS BALANCE ERROR: (1)-(2) = -0.2408E-08
(4) RELATIVE MASS BALANCE ERROR: ABS(3)/(ABS(1)+ABS(2)) = 0.6510E-11

TIME STEP NO. 24 HAS BEEN COMPLETED TOTAL ITERATION NUMBER = 82

****
* ELAPSED SIMULATION TIME = 0.8640E+07 *
****

CUMULATIVE NUMBER OF COMPUTATIONAL TIME STEPS = 26

CURRENT VALUE OF COMPUTATIONAL TIME STEP (DT) = 0.1471E+07

SUMMARY OF NONLINEAR ITERATION USING RELATIVE CONVERGENCE CRITERION

ITERATION	NUMBER OF NON-CONVERGENT NODAL VALUES	MAXIMUM RELATIVE ERROR	NODAL UNKNOWN NUMBER
1	6	0.179541E-01	20
2	6	0.170930E-01	20
3	0	0.780098E-04	19

****
* SIMULATION RESULTS *
****

NODE	PRES. (PH. 1)	SAT. (PH. 1)	SAT. (PH. 2)	PRES. (PH. 2)	SAT. (PH. 3)	PRES. (PH. 3)
1	0.8849E+05	0.2008E+00	0.1803E+00	0.9746E+05	0.6189E+00	0.1000E+06
2	0.8855E+05	0.2008E+00	0.1891E+00	0.9752E+05	0.6101E+00	0.1000E+06
3	0.8859E+05	0.2008E+00	0.1940E+00	0.9756E+05	0.6052E+00	0.1000E+06
4	0.8861E+05	0.2008E+00	0.1967E+00	0.9758E+05	0.6025E+00	0.1000E+06
5	0.8862E+05	0.2008E+00	0.1983E+00	0.9759E+05	0.6009E+00	0.1000E+06
6	0.8862E+05	0.2008E+00	0.1988E+00	0.9759E+05	0.6003E+00	0.1000E+06
7	0.8879E+05	0.2147E+00	0.1404E+00	0.9726E+05	0.6448E+00	0.9999E+05
8	0.9341E+05	0.2008E+00	0.7559E-21	0.9341E+05	0.7992E+00	0.9999E+05
9	0.9341E+05	0.2008E+00	0.7304E-24	0.9341E+05	0.7992E+00	0.1000E+06
10	0.9341E+05	0.2008E+00	-0.1167E-28	0.9341E+05	0.7992E+00	0.1000E+06
11	0.9341E+05	0.2008E+00	-0.4507E-09	0.9341E+05	0.7992E+00	0.1000E+06
12	0.9342E+05	0.2008E+00	-0.4891E-09	0.9342E+05	0.7992E+00	0.1000E+06
13	0.9342E+05	0.2008E+00	-0.4832E-09	0.9342E+05	0.7992E+00	0.1000E+06
14	0.9342E+05	0.2008E+00	-0.4851E-09	0.9342E+05	0.7992E+00	0.1000E+06
15	0.9342E+05	0.2008E+00	0.1908E-08	0.9342E+05	0.7992E+00	0.1000E+06
16	0.9342E+05	0.2008E+00	0.6359E-30	0.9342E+05	0.7992E+00	0.1000E+06
17	0.9342E+05	0.2008E+00	0.6911E-30	0.9342E+05	0.7992E+00	0.1000E+06
18	0.9343E+05	0.2008E+00	0.7120E-30	0.9343E+05	0.7992E+00	0.1000E+06
19	0.9349E+05	0.2044E+00	0.6397E-28	0.9349E+05	0.7956E+00	0.1000E+06
20	0.9755E+05	0.7533E+00	-0.3052E-29	0.9755E+05	0.2467E+00	0.1000E+06

SUMMARY OF MASS BALANCE COMPUTATION FOR FLOW SIMULATION

WATER

(1) CUMULATIVE (INFLOW-OUTFLOW) MASS = 0.5005E+01
(2) CUMULATIVE MASS STORAGE CHANGES = 0.5009E+01
(3) MASS BALANCE ERROR: (1)-(2) = -0.4418E-02
(4) RELATIVE MASS BALANCE ERROR: ABS(3)/(ABS(1)+ABS(2)) = 0.4412E-03

NAPL

(1) CUMULATIVE (INFLOW-OUTFLOW) MASS = 0.1849E+03
(2) CUMULATIVE MASS STORAGE CHANGES = 0.1849E+03
(3) MASS BALANCE ERROR: (1)-(2) = -0.2411E-08
(4) RELATIVE MASS BALANCE ERROR: ABS(3)/(ABS(1)+ABS(2)) = 0.6519E-11

TIME STEP NO. 26 HAS BEEN COMPLETED TOTAL ITERATION NUMBER = 90

****
* ELAPSED SIMULATION TIME = 0.1167E+08 *
****

CUMULATIVE NUMBER OF COMPUTATIONAL TIME STEPS = 30

CURRENT VALUE OF COMPUTATIONAL TIME STEP (DT) = 0.8640E+05
SUMMARY OF NONLINEAR ITERATION USING RELATIVE CONVERGENCE CRITERION

ITERATION	NUMBER OF NON-CONVERGENT NODAL VALUES	MAXIMUM RELATIVE ERROR	NODAL UNKNOWN NUMBER
1	1	0.153708E-02	20
2	0	0.136368E-07	58

****
* SIMULATION RESULTS *
****

NODE	PRES. (PH. 1)	SAT. (PH. 1)	SAT. (PH. 2)	PRES. (PH. 2)	SAT. (PH. 3)	PRES. (PH. 3)
1	0.8842E+05	0.2008E+00	0.1709E+00	0.9739E+05	0.6283E+00	0.1000E+06
2	0.8845E+05	0.2008E+00	0.1755E+00	0.9742E+05	0.6237E+00	0.1000E+06
3	0.8849E+05	0.2008E+00	0.1808E+00	0.9746E+05	0.6184E+00	0.1000E+06
4	0.8853E+05	0.2008E+00	0.1858E+00	0.9750E+05	0.6134E+00	0.1000E+06
5	0.8856E+05	0.2008E+00	0.1901E+00	0.9753E+05	0.6091E+00	0.1000E+06
6	0.8860E+05	0.2009E+00	0.1952E+00	0.9757E+05	0.6040E+00	0.1000E+06
7	0.8896E+05	0.2093E+00	0.1995E+00	0.9762E+05	0.5912E+00	0.1000E+06
8	0.9341E+05	0.2009E+00	0.7559E-21	0.9341E+05	0.7991E+00	0.9999E+05
9	0.9341E+05	0.2009E+00	0.7304E-24	0.9341E+05	0.7991E+00	0.1000E+06
10	0.9341E+05	0.2009E+00	-0.1167E-28	0.9341E+05	0.7991E+00	0.1000E+06
11	0.9341E+05	0.2009E+00	-0.4507E-09	0.9341E+05	0.7991E+00	0.1000E+06
12	0.9342E+05	0.2009E+00	-0.4891E-09	0.9342E+05	0.7991E+00	0.1000E+06
13	0.9342E+05	0.2009E+00	-0.4832E-09	0.9342E+05	0.7991E+00	0.1000E+06
14	0.9342E+05	0.2009E+00	-0.4851E-09	0.9342E+05	0.7991E+00	0.1000E+06
15	0.9342E+05	0.2009E+00	0.1908E-08	0.9342E+05	0.7991E+00	0.1000E+06
16	0.9342E+05	0.2009E+00	0.6359E-30	0.9342E+05	0.7991E+00	0.1000E+06
17	0.9343E+05	0.2009E+00	0.6911E-30	0.9343E+05	0.7991E+00	0.1000E+06
18	0.9343E+05	0.2009E+00	0.7120E-30	0.9343E+05	0.7991E+00	0.1000E+06
19	0.9350E+05	0.2050E+00	0.6397E-28	0.9350E+05	0.7950E+00	0.1000E+06
20	0.9755E+05	0.7533E+00	-0.3052E-29	0.9755E+05	0.2467E+00	0.1000E+06

SUMMARY OF MASS BALANCE COMPUTATION FOR FLOW SIMULATION

WATER

(1) CUMULATIVE (INFLOW-OUTFLOW) MASS = 0.4394E+01
(2) CUMULATIVE MASS STORAGE CHANGES = 0.4399E+01
(3) MASS BALANCE ERROR: (1)-(2) = -0.4450E-02
(4) RELATIVE MASS BALANCE ERROR: ABS(3)/(ABS(1)+ABS(2)) = 0.5061E-03

NAPL

(1) CUMULATIVE (INFLOW-OUTFLOW) MASS = 0.1849E+03
(2) CUMULATIVE MASS STORAGE CHANGES = 0.1849E+03
(3) MASS BALANCE ERROR: (1)-(2) = -0.2001E-09
(4) RELATIVE MASS BALANCE ERROR: ABS(3)/(ABS(1)+ABS(2)) = 0.5410E-12

TIME STEP NO. 30 HAS BEEN COMPLETED TOTAL ITERATION NUMBER = 98

****
* ELAPSED SIMULATION TIME = 0.3591E+08 *
****

CUMULATIVE NUMBER OF COMPUTATIONAL TIME STEPS = 40

CURRENT VALUE OF COMPUTATIONAL TIME STEP (DT) = 0.8640E+07

SUMMARY OF NONLINEAR ITERATION USING RELATIVE CONVERGENCE CRITERION

ITERATION	NUMBER OF NON-CONVERGENT NODAL VALUES	MAXIMUM RELATIVE ERROR	NODAL UNKNOWN NUMBER

1	3	0.508405E-02	23
2	0	0.210190E-04	23

****
* SIMULATION RESULTS *
****

NODE	PRES. (PH. 1)	SAT. (PH. 1)	SAT. (PH. 2)	PRES. (PH. 2)	SAT. (PH. 3)	PRES. (PH. 3)
1	0.8840E+05	0.2008E+00	0.1682E+00	0.9737E+05	0.6309E+00	0.1000E+06
2	0.8840E+05	0.2008E+00	0.1683E+00	0.9737E+05	0.6309E+00	0.1000E+06
3	0.8840E+05	0.2008E+00	0.1683E+00	0.9737E+05	0.6309E+00	0.1000E+06
4	0.8840E+05	0.2008E+00	0.1684E+00	0.9737E+05	0.6308E+00	0.1000E+06
5	0.8840E+05	0.2008E+00	0.1686E+00	0.9737E+05	0.6306E+00	0.1000E+06
6	0.8840E+05	0.2008E+00	0.1690E+00	0.9737E+05	0.6302E+00	0.1000E+06
7	0.8842E+05	0.2009E+00	0.1719E+00	0.9739E+05	0.6272E+00	0.1000E+06
8	0.8873E+05	0.2178E+00	0.1151E+00	0.9709E+05	0.6672E+00	0.1000E+06
9	0.9341E+05	0.2008E+00	0.7304E-24	0.9341E+05	0.7992E+00	0.1000E+06
10	0.9341E+05	0.2008E+00	-0.1167E-28	0.9341E+05	0.7992E+00	0.1000E+06
11	0.9341E+05	0.2008E+00	-0.4507E-09	0.9341E+05	0.7992E+00	0.1000E+06
12	0.9342E+05	0.2008E+00	-0.4891E-09	0.9342E+05	0.7992E+00	0.1000E+06
13	0.9342E+05	0.2008E+00	-0.4832E-09	0.9342E+05	0.7992E+00	0.1000E+06
14	0.9342E+05	0.2008E+00	-0.4851E-09	0.9342E+05	0.7992E+00	0.1000E+06
15	0.9342E+05	0.2008E+00	0.1908E-08	0.9342E+05	0.7992E+00	0.1000E+06
16	0.9342E+05	0.2008E+00	0.6359E-30	0.9342E+05	0.7992E+00	0.1000E+06
17	0.9343E+05	0.2008E+00	0.6911E-30	0.9343E+05	0.7992E+00	0.1000E+06
18	0.9343E+05	0.2008E+00	0.7120E-30	0.9343E+05	0.7992E+00	0.1000E+06
19	0.9350E+05	0.2047E+00	0.6397E-28	0.9350E+05	0.7953E+00	0.1000E+06
20	0.9755E+05	0.7533E+00	-0.3052E-29	0.9755E+05	0.2467E+00	0.1000E+06

SUMMARY OF MASS BALANCE COMPUTATION FOR FLOW SIMULATION

WATER

(1) CUMULATIVE (INFLOW-OUTFLOW) MASS = 0.5511E+01
(2) CUMULATIVE MASS STORAGE CHANGES = 0.5516E+01
(3) MASS BALANCE ERROR: (1)-(2) = -0.5225E-02
(4) RELATIVE MASS BALANCE ERROR: ABS(3)/(ABS(1)+ABS(2)) = 0.4739E-03

NAPL

(1) CUMULATIVE (INFLOW-OUTFLOW) MASS = 0.1849E+03
(2) CUMULATIVE MASS STORAGE CHANGES = 0.1849E+03
(3) MASS BALANCE ERROR: (1)-(2) = -0.1390E-07
(4) RELATIVE MASS BALANCE ERROR: ABS(3)/(ABS(1)+ABS(2)) = 0.3759E-10

TIME STEP NO. 40 HAS BEEN COMPLETED TOTAL ITERATION NUMBER = 128

***** SAMFT1D HAS SOLVED THE PROBLEM *****

****
*** CPU TIME USED: 145.2 SECS. ***
****

10.6 MULTIPHASE PHASE TRANSPORT

10.6.1 Input Data

Input data for this multiphase transport example is presented in Table 10.6.1. The problem corresponds to the example three-phase flow problem of Section 10.5, and has been used as a test case (See Section 4.5.2.1). Note here that the automatic mesh-centered grid generation option is used by setting IBCGR equal to 0. Because the output control parameter IPRD is set equal to 0, the mesh data and initial condition data occur in the printed output. The boundary conditions are (i) flux conditions on the top surface with water injection only; (ii) no boundary conditions specified on the bottom boundary. Then the code will set a zero dispersive flux boundary on the bottom surface.

Table 10.6.1 Input Data for the Multiphase Transport Simulation Problem

```
 1    1                                                                    GROUP 1
 TEST OF SAMFT1D MODULE FOR MULTIPHASE TRANSPORT                           GROUP 2
 0    3    3    0    1    0    2   40   20    1    1    1                 GROUP 3
 0   10    1        .01      1.0E0 9.8066E00 1.00000E5      .001    0.001 GROUP 4
 1    0    8    0    0    0   10   10    1    1    1    0    0            GROUP 5
    0.0   1.00E09     .50E07    1                                         GROUP 6C
    0.0                                                                  GROUP 8
1.00E00     .58E00     3.3E00        0.3    1.5E03                       GROUP 10A
1.00E-5     .10E-6     1.0E-4                                            GROUP 10B
0.00E00     0.1E-3                                                       GROUP 10C
0.10E04     9.5E02   1.177E00                                           GROUP 10D
0.00E01     0.25E0      .01E00                                          GROUP 10E
 1    0       1.E0     0                                                GROUP 11
 1   20    1         10.                                                GROUP 12
 0    1    0    0                                                       GROUP 13
 1    1   0.00E00 3.246E-6                                             GROUP 14B
 1        .01    47.937                                                GROUP 17A
 2        .01    47.937                                                GROUP 17A
 3        .01    47.937                                                GROUP 17A
 4        .01    47.951                                                GROUP 17A
 5        .01    47.994                                                GROUP 17A
 6        .01    48.549                                                GROUP 17A
 7        .01    47.937                                                GROUP 17A
 8        .01    23.142                                                GROUP 17A
 1        .00                                                           GROUP 18
 1        0.5  0.50E-05                                                GROUP 19
 2        0.3  0.50E-05                                                GROUP 19
 3        0.2  0.00E-04                                                GROUP 19
 2                                                                      GROUP 20
 1   10                                                                 GROUP 21
```

10.6.2 Output

The output from the line printer for this multiphase transport problem is displayed in Table 10.6.2. This output, which corresponds to input data in Table 10.6.1, consists of the following categories of information:

1. Brief summary of control input data.
2. List of generated time values.
3. Summary of solute and material properties.
4. Mesh data.
5. Prescribed boundary condition data.
6. Initial condition data.
7. Time and time-step number.
8. Node numbers and nodal values of solute concentrations in water, NAPL, air and solid phases, and precipitated mass, corresponding to the given time value.
9. Mass balance budget.

Note that information in categories 6 through 9 are repeated for each time step.

Table 10.6.2. Output for the Multiphase Transport Simulation Problem.

```
PROBLEM IDENTIFICATION NUMBER =     1

PROBLEM TITLE
-------------------------------------------------------------------------------

    TEST OF SAMFT1D MODULE FOR MULTIPHASE TRANSPORT

-------------------------------------------------------------------------------



PROBLEM SPECIFICATION PARAMETERS
--------------------------------
MODEL OPTION PARAMETER ...................(IMODL) =     0
  NOTE:  IMODL = 0 FOR SOLUTE TRANSPORT ONLY
               = 1 FOR FLUID FLOW ONLY
               = 2 FOR COUPLED FLOW AND TRANSPORT
TOTAL NUMBER OF FLUID PHASES..... (NTPHAS) =     3
NUMBER OF ACTIVE FLUID PHASES..... (NMPHAS) =     3
HYSTERESIS CONSIDERATION (1=YES,0=NO).....(IHYST) =     0
TOTAL NUMBER OF PRIMARY DEPENDENT VARIABLES(NVAR) =     1
STEADY STATE SIMULATION(1=YES, 0=NO).....(ISSTA) =     0
TIME STEP GENERATION INDEX (1=YES, 0=NO) .(ITSGN) =     2
NUMBER OF TIME STEPS .....................(NTS) =    40
TOTAL NUMBER OF ELEMENTS .....................(NE) =    20
NUMBER OF POROUS MATERIALS .................(NMAT) =     1
SOIL CONSTITUTIVE DATA(0=FUNCTION,1=TABLE)(KPROP) =     1
INITIAL CONDITION NON-UNIFORMITY INDEX ....(NONU) =     1


INPUT / OUTPUT CONTROL PARAMETERS
---------------------------------
VELOCITY/INPUT.........................(NVREAD) =     1
BOUNDARY NODE DATA READ (1=YES, 0=NO)....(IOUTLT) =     0
NUMBER OF NODES FOR WHICH I.C. ARE READ....(NPIN) =     8
OUTPUT REQUIREMENT INDICATOR:
 (0=ALL DATA, 1=NO ELEMENT DATA,
  2=NO DATA, 3=NO MESH AND I.C. DATA.......(IPRD) =     0
UNIT 9 OUTPUT OF VEL / SAT (1=YES, 0=NO).(NVWRIT) =     0
VELOCITY PRINTOUT CONTROL INDEX.....(NVPR) =     0
UNIT 10 AND/OR 11 FOR PLOT (0=NO,>0=YES)..(NPLOT) =    10
TIME STEP INCREMENT FOR OUTPUT PRINT OUT..(NSTEP) =    10
OBSERVATION NODE INDEX...................(IOBSND) =     1
MASS BALANCE TO BE PERFORMED (1=YES,0=NO).(IMBAL) =     1
UNIT 8 OUTPUT OF HEAD/CONC (1=YES, 0=NO).(NOWRIT) =     1
PRINT CHECK OPTION INDEX.................(IPRCHK) =     0
NO. OF SPECIFIED T VALUES FOR PRINTOUT...(NPCORN) =     0

TIME STEP. PARAMETER FOR TRANSPORT SIMULATION.(IKALL) =     0


*** LIST OF GENERATED TIME VALUES ***
-------------------------------------

 0.500E+07 0.100E+08 0.150E+08 0.200E+08 0.250E+08 0.300E+08 0.350E+08 0.400E+08
 0.450E+08 0.500E+08 0.550E+08 0.600E+08 0.650E+08 0.700E+08 0.750E+08 0.800E+08
 0.850E+08 0.900E+08 0.950E+08 0.100E+09 0.105E+09 0.110E+09 0.115E+09 0.120E+09
 0.125E+09 0.130E+09 0.135E+09 0.140E+09 0.145E+09 0.150E+09 0.155E+09 0.160E+09
 0.165E+09 0.170E+09 0.175E+09 0.180E+09 0.185E+09 0.190E+09 0.195E+09 0.200E+09
```

```
DEFAULT INITIAL CONDITION FOR TRANSPORT PROBLEM
-----------------------------------------------

PRESCRIBED INITIAL CONCENTRATION VALUE....(CIDFAL) =  0.0000E+00


TRANSPORT PROPERTIES OF POROUS MEDIA
------------------------------------


MATERIAL NUMBER (I):    1

LONGITUDINAL DISPERSIVITY.............(PROPJ(I,1)) =  0.1000E+01
TORTUOSITY FACTOR..................... ..(PROPJ(I,2)) =  0.5800E+00
EXPONENT OF MOL. DIFF. COEFF..........(PROPJ(I,3)) =  0.3300E+01
EFFECTIVE POROSITY(0 FOR STEADY STATE)(PROPJ(I,4)) =  0.3000E+00
BULK DENSITY..........................(PROPJ(I,5)) =  0.1500E+04

MOLECULAR DIFFUSION COEFFICIENT OF PHASE 1 THROUGH NTPHAS
---------------------------------------------------------

      0.100E-08      0.100E-08      0.100E-04


SOLUTE PROPERTIES
-----------------

MATERIAL NUMBER (I) :    1
--------------------
DECAY COEFFICIENT ..................... (RPROP(I,1)) =  0.0000E+00
DISTRIBUTION COEF. FOR PH.#1 & SOIL.. (RPROP(I,2)) =  0.1000E-03
DENSITY OF FLUID PHASE #  1  ..................... =  0.1000E+04
DENSITY OF FLUID PHASE #  2  ..................... =  0.9500E+03
DENSITY OF FLUID PHASE #  3  ..................... =  0.1177E+01

FLUID-PAIR PART. COEF. & SOLUBILITY
-----------------------------------
SOLUTE PART. COEF FOR 1 & 2 PHASES...... PCOEF(1)) =  0.0000E+00
SOLUTE PART. COEF FOR 1 & 3 PHASES...... PCOEF(2)) =  0.2500E+00
SOLUBILITY LIMIT IN WATER PHASE......... PCOEF(3)) =  0.1000E-01


GRID GENERATION PARAMETERS
--------------------------
NUMBER OF SOIL LAYERS.....................(NLAYER) =    1
PARAMETER INDICATING THE GRID TYPE (IBCGR)
(0=MESH-CENTERED (F.E.), 1=BLOCK-CENTERED(F.D.))...=    0
CROSS-SECTIONAL AREA OF THE SOIL COLUMN....(ACROS) =  0.1000E+01
PARAMETER INDICATING GRID ORIENTATION.....(IHORGR) =    0
IHORGR=0 FOR VERTIAL FLOW, IHORGR=1 FOR HORIZONTAL FLOW
PARAMETER FOR BC TREATMENT SELECTION OF MULTIPHASE FLOW
IBCGRD=0, NO SPECIAL TREATMENT
IBCGRD=1, BIG NUMBER TREATMENT............(IBCGRD) =    0


LAYERED GRID DATA
-----------------


LAYER NUMBER :    1
------------------
NO. OF ELEMENTS (OR GRID BLOCKS) ..........(NELM) =   20
MATERIAL NUMBER ...........................(IMATL) =    1
LAYER THICKNESS............................(THL) =  0.1000E+02


************************************************
*** MESH-CENTERED FINITE ELEMENT GRID IS USED ***
```

```
************************************************
```

NODE	Z-COOR.	NODE	Z-COOR.	NODE	Z-COOR.	NODE	Z-COOR.
1	0.00	2	0.50	3	1.00	4	1.50
5	2.00	6	2.50	7	3.00	8	3.50
9	4.00	10	4.50	11	5.00	12	5.50
13	6.00	14	6.50	15	7.00	16	7.50
17	8.00	18	8.50	19	9.00	20	9.50
21	10.00						

```
BOUNDARY CONDITION DATA
-----------------------

NO. OF STEADY DIRICHLET BOUNDARY CONDITIONS....(NBTO) =    0
NO. OF STEADY FLUX BOUNDARY CONDITIONS..... (NDFLUX) =    1
NO. OF TRANSIENT DIRICHLET BOUNDARY CONDITIONS(NBHVAR)=    0
NO. OF TRANSIENT FLUX BOUNDARY CONDITIONS... (NBFVAR) =    0


STEADY-STATE FLUX BOUNDARY CONDITIONS
-------------------------------------
```

INDEX	NODE NO.	MDEGF(I)	FLUID FLUX	SOLUTE FLUX
1	1	1	3.2460E-06	0.0000E+00

```
TRANSPORT SIMULATION CONTROL DATA
---------------------------------

STEADY-STATE VELOCITY FIELD (0=NO,1=YES)..(IVSTED) =    1
UPSTREAM FACTOR .............................(WFAC) =  0.00E+00


DEFAULT PHASE SATURATION AND DARCY VELOCITY VALUES
--------------------------------------------------

FLUID PHASE NUMBER    1
----------------------
PHASE SATURATION (DEFAULT VALUE)..... =  0.5000E+00
DEFAULT VALUE OF DARCY VELOCITY ..... =  0.5000E-05

FLUID PHASE NUMBER    2
----------------------
PHASE SATURATION (DEFAULT VALUE)..... =  0.3000E+00
DEFAULT VALUE OF DARCY VELOCITY ..... =  0.5000E-05

FLUID PHASE NUMBER    3
----------------------
PHASE SATURATION (DEFAULT VALUE)..... =  0.2000E+00
DEFAULT VALUE OF DARCY VELOCITY ..... =  0.0000E+00


LIST OF OBSERVATION NODES
-------------------------

1    10



**************************
* INITIAL CONDITION DATA *
**************************
```

NODE	CONC. (Cw)	PRECIP. MASS
1	0.1000E-01	0.4796E+02
2	0.1000E-01	0.4796E+02
3	0.1000E-01	0.4796E+02
4	0.1000E-01	0.4796E+02
5	0.1000E-01	0.4797E+02
6	0.1000E-01	0.4803E+02
7	0.1000E-01	0.4904E+02
8	0.1000E-01	0.4408E+02
9	0.0000E+00	0.0000E+00
10	0.0000E+00	0.0000E+00
11	0.0000E+00	0.0000E+00
12	0.0000E+00	0.0000E+00
13	0.0000E+00	0.0000E+00
14	0.0000E+00	0.0000E+00
15	0.0000E+00	0.0000E+00
16	0.0000E+00	0.0000E+00
17	0.0000E+00	0.0000E+00
18	0.0000E+00	0.0000E+00
19	0.0000E+00	0.0000E+00
20	0.0000E+00	0.0000E+00
21	0.0000E+00	0.0000E+00

****
* ELAPSED SIMULATION TIME = 0.5000E+08 *
****

CUMULATIVE NUMBER OF COMPUTATIONAL TIME STEPS = 10

CURRENT VALUE OF COMPUTATIONAL TIME STEP (DT) = 0.5000E+07

****
* SIMULATION RESULTS *
****

NODE	(Cw)	(Cn)	(Ca)	(Cs)	PRECIP. MASS
1	0.1000E-01	0.0000E+00	0.2500E-02	0.1000E-02	0.4162E+02
2	0.1000E-01	0.0000E+00	0.2500E-02	0.1000E-02	0.4796E+02
3	0.1000E-01	0.0000E+00	0.2500E-02	0.1000E-02	0.4796E+02
4	0.1000E-01	0.0000E+00	0.2500E-02	0.1000E-02	0.4796E+02
5	0.1000E-01	0.0000E+00	0.2500E-02	0.1000E-02	0.4797E+02
6	0.1000E-01	0.0000E+00	0.2500E-02	0.1000E-02	0.4803E+02
7	0.1000E-01	0.0000E+00	0.2500E-02	0.1000E-02	0.4904E+02
8	0.1000E-01	0.0000E+00	0.2500E-02	0.1000E-02	0.4202E+02
9	0.8412E-02	0.0000E+00	0.2103E-02	0.8412E-03	0.0000E+00
10	0.6477E-02	0.0000E+00	0.1619E-02	0.6477E-03	0.0000E+00
11	0.4496E-02	0.0000E+00	0.1124E-02	0.4496E-03	0.0000E+00
12	0.2780E-02	0.0000E+00	0.6949E-03	0.2780E-03	0.0000E+00
13	0.1513E-02	0.0000E+00	0.3782E-03	0.1513E-03	0.0000E+00
14	0.7168E-03	0.0000E+00	0.1792E-03	0.7168E-04	0.0000E+00
15	0.2923E-03	0.0000E+00	0.7306E-04	0.2923E-04	0.0000E+00
16	0.1016E-03	0.0000E+00	0.2539E-04	0.1016E-04	0.0000E+00
17	0.2994E-04	0.0000E+00	0.7484E-05	0.2994E-05	0.0000E+00

18	0.7535E-05	0.0000E+00	0.1884E-05	0.7535E-06	0.0000E+00
19	0.1632E-05	0.0000E+00	0.4081E-06	0.1632E-06	0.0000E+00
20	0.2621E-06	0.0000E+00	0.6552E-07	0.2621E-07	0.0000E+00
21	0.3483E-07	0.0000E+00	0.8707E-08	0.3483E-08	0.0000E+00

SUMMARY OF MASS BALANCE COMPUTATION FOR TRANSPORT SIMULATION

MASS BALANCE RESULTS OVER A TIME STEP

(1) NET SOLUTE MASS TRANSFERED TO PRECIP. PHASE	=	-0.2042E+00
(2) NET DECAYED SOLUTE MASS	=	0.0000E+00
(3) NET (INFLOW-OUTFLOW) SOLUTE MASS	=	-0.5522E-06
(4) NET SOLUTE MASS STORAGE CHANGES	=	0.2042E+00
(5) MASS BALANCE ERROR:	=	0.1853E-06
(6) RELATIVE MASS BALANCE ERROR:	=	0.9803E-09

CUMULATIVE MASS BALANCE RESULTS

(1) CUMULATIVE SOLUTE MASS TRANSFERED TO PRECIP. PHASE	=	-0.2616E+01
(2) CUMULATIVE DECAYED SOLUTE MASS	=	0.0000E+00
(3) CUMULATIVE (INFLOW-OUTFLOW) SOLUTE MASS	=	-0.8232E-06
(4) CUMULATIVE SOLUTE MASS STORAGE CHANGES	=	0.2616E+01
(5) CUMULATIVE MASS BALANCE ERROR	=	0.2753E-06
(6) CUMULATIVE RELATIVE MASS BALANCE ERROR	=	0.1438E-08

****
* ELEMENTAL SATURATION AND VELOCITIES *
****

ELEM.	SAT. (PH. 1)	SAT. (PH. 2)	SAT. (PH. 3)	VELOC.(PH. 1)	VELOC.(PH. 2)	VELOC.(PH. 3)
1	0.200800E+00	0.1683E+00	0.6309E+00	0.317100E-08	0.7522E-17	0.135000E-13
2	0.200800E+00	0.1683E+00	0.6309E+00	0.317100E-08	0.3146E-16	0.128400E-13
3	0.200800E+00	0.1683E+00	0.6309E+00	0.317100E-08	0.9095E-16	0.127100E-13
4	0.200800E+00	0.1683E+00	0.6309E+00	0.317100E-08	0.2171E-15	0.115100E-13
5	0.200800E+00	0.1684E+00	0.6308E+00	0.317100E-08	0.4436E-15	0.108500E-13
6	0.200800E+00	0.1699E+00	0.6292E+00	0.317100E-08	0.0000E+00	0.101800E-13
7	0.209400E+00	0.1312E+00	0.6594E+00	0.317100E-08	0.0000E+00	0.951800E-14
8	0.209400E+00	0.4552E-03	0.7451E+00	0.317100E-08	0.0000E+00	0.885800E-14
9	0.200800E+00	0.0000E+00	0.7992E+00	0.317100E-08	0.0000E+00	0.819200E-14
10	0.200800E+00	0.0000E+00	0.7992E+00	0.317100E-08	0.0000E+00	0.752700E-14
11	0.200800E+00	0.0000E+00	0.7992E+00	0.317100E-08	0.0000E+00	0.686300E-14
12	0.200800E+00	0.0000E+00	0.7992E+00	0.317100E-08	0.0000E+00	0.618900E-14
13	0.200800E+00	0.0000E+00	0.7992E+00	0.317100E-08	0.0000E+00	0.553300E-14
14	0.200800E+00	0.0000E+00	0.7992E+00	0.317100E-08	0.0000E+00	0.486800E-14
15	0.200800E+00	0.0000E+00	0.7992E+00	0.317100E-08	0.0000E+00	0.420300E-14
16	0.200800E+00	0.0000E+00	0.7992E+00	0.317100E-08	0.0000E+00	0.353700E-14
17	0.200800E+00	0.0000E+00	0.7992E+00	0.317100E-08	0.0000E+00	0.287100E-14
18	0.201000E+00	0.0000E+00	0.7990E+00	0.317100E-08	0.0000E+00	0.220500E-14
19	0.250600E+00	0.0000E+00	0.7494E+00	0.317100E-08	0.0000E+00	0.153900E-14
20	0.649900E+00	0.0000E+00	0.3501E+00	0.317100E-08	0.0000E+00	-0.107900E-10

TIME STEP NO. 10 HAS BEEN COMPLETED TOTAL ITERATION NUMBER = 0

****
* ELAPSED SIMULATION TIME = 0.1000E+09 *
****

CUMULATIVE NUMBER OF COMPUTATIONAL TIME STEPS = 20

CURRENT VALUE OF COMPUTATIONAL TIME STEP (DT) = 0.5000E+07

****
* SIMULATION RESULTS *
****

NODE	(Cw)	(Cn)	(Ca)	(Cs)	PRECIP. MASS
1	0.1000E-01	0.0000E+00	0.2500E-02	0.1000E-02	0.3528E+02
2	0.1000E-01	0.0000E+00	0.2500E-02	0.1000E-02	0.4796E+02
3	0.1000E-01	0.0000E+00	0.2500E-02	0.1000E-02	0.4796E+02
4	0.1000E-01	0.0000E+00	0.2500E-02	0.1000E-02	0.4796E+02
5	0.1000E-01	0.0000E+00	0.2500E-02	0.1000E-02	0.4797E+02
6	0.1000E-01	0.0000E+00	0.2500E-02	0.1000E-02	0.4803E+02
7	0.1000E-01	0.0000E+00	0.2500E-02	0.1000E-02	0.4904E+02
8	0.1000E-01	0.0000E+00	0.2500E-02	0.1000E-02	0.4142E+02
9	0.9234E-02	0.0000E+00	0.2308E-02	0.9234E-03	0.0000E+00
10	0.8212E-02	0.0000E+00	0.2053E-02	0.8212E-03	0.0000E+00
11	0.6987E-02	0.0000E+00	0.1747E-02	0.6987E-03	0.0000E+00
12	0.5657E-02	0.0000E+00	0.1414E-02	0.5657E-03	0.0000E+00
13	0.4338E-02	0.0000E+00	0.1085E-02	0.4338E-03	0.0000E+00
14	0.3139E-02	0.0000E+00	0.7847E-03	0.3139E-03	0.0000E+00
15	0.2135E-02	0.0000E+00	0.5336E-03	0.2135E-03	0.0000E+00
16	0.1360E-02	0.0000E+00	0.3399E-03	0.1360E-03	0.0000E+00
17	0.8084E-03	0.0000E+00	0.2021E-03	0.8084E-04	0.0000E+00
18	0.4461E-03	0.0000E+00	0.1115E-03	0.4461E-04	0.0000E+00
19	0.2243E-03	0.0000E+00	0.5608E-04	0.2243E-04	0.0000E+00
20	0.9535E-04	0.0000E+00	0.2384E-04	0.9535E-05	0.0000E+00
21	0.4924E-04	0.0000E+00	0.1231E-04	0.4924E-05	0.0000E+00

SUMMARY OF MASS BALANCE COMPUTATION FOR TRANSPORT SIMULATION

MASS BALANCE RESULTS OVER A TIME STEP

(1) NET SOLUTE MASS TRANSFERED TO PRECIP. PHASE	=	-0.1798E+00
(2) NET DECAYED SOLUTE MASS	=	0.0000E+00
(3) NET (INFLOW-OUTFLOW) SOLUTE MASS	=	-0.7807E-03
(4) NET SOLUTE MASS STORAGE CHANGES	=	0.1791E+00
(5) MASS BALANCE ERROR:	=	0.1254E-03
(6) RELATIVE MASS BALANCE ERROR:	=	0.6635E-06

CUMULATIVE MASS BALANCE RESULTS

(1) CUMULATIVE SOLUTE MASS TRANSFERED TO PRECIP. PHASE	=	-0.4500E+01
(2) CUMULATIVE DECAYED SOLUTE MASS	=	0.0000E+00
(3) CUMULATIVE (INFLOW-OUTFLOW) SOLUTE MASS	=	-0.2092E-02
(4) CUMULATIVE SOLUTE MASS STORAGE CHANGES	=	0.4498E+01
(5) CUMULATIVE MASS BALANCE ERROR	=	0.3904E-03
(6) CUMULATIVE RELATIVE MASS BALANCE ERROR	=	0.2019E-05

****
* ELEMENTAL SATURATION AND VELOCITIES *
****

ELEM.	SAT. (PH. 1)	SAT. (PH. 2)	SAT. (PH. 3)	VELOC.(PH. 1)	VELOC.(PH. 2)	VELOC.(PH. 3)
1	0.200800E+00	0.1683E+00	0.6309E+00	0.317100E-08	0.7522E-17	0.135000E-13
2	0.200800E+00	0.1683E+00	0.6309E+00	0.317100E-08	0.3146E-16	0.128400E-13
3	0.200800E+00	0.1683E+00	0.6309E+00	0.317100E-08	0.9095E-16	0.127100E-13
4	0.200800E+00	0.1683E+00	0.6309E+00	0.317100E-08	0.2171E-15	0.115100E-13
5	0.200800E+00	0.1684E+00	0.6308E+00	0.317100E-08	0.4436E-15	0.108500E-13
6	0.200800E+00	0.1699E+00	0.6292E+00	0.317100E-08	0.0000E+00	0.101800E-13
7	0.209400E+00	0.1312E+00	0.6594E+00	0.317100E-08	0.0000E+00	0.951800E-14
8	0.209400E+00	0.4552E-03	0.7451E+00	0.317100E-08	0.0000E+00	0.885800E-14
9	0.200800E+00	0.0000E+00	0.7992E+00	0.317100E-08	0.0000E+00	0.819200E-14
10	0.200800E+00	0.0000E+00	0.7992E+00	0.317100E-08	0.0000E+00	0.752700E-14
11	0.200800E+00	0.0000E+00	0.7992E+00	0.317100E-08	0.0000E+00	0.686300E-14
12	0.200800E+00	0.0000E+00	0.7992E+00	0.317100E-08	0.0000E+00	0.618900E-14
13	0.200800E+00	0.0000E+00	0.7992E+00	0.317100E-08	0.0000E+00	0.553300E-14
14	0.200800E+00	0.0000E+00	0.7992E+00	0.317100E-08	0.0000E+00	0.486800E-14
15	0.200800E+00	0.0000E+00	0.7992E+00	0.317100E-08	0.0000E+00	0.420300E-14
16	0.200800E+00	0.0000E+00	0.7992E+00	0.317100E-08	0.0000E+00	0.353700E-14
17	0.200800E+00	0.0000E+00	0.7992E+00	0.317100E-08	0.0000E+00	0.287100E-14
18	0.201000E+00	0.0000E+00	0.7990E+00	0.317100E-08	0.0000E+00	0.220500E-14
19	0.250600E+00	0.0000E+00	0.7494E+00	0.317100E-08	0.0000E+00	0.153900E-14
20	0.649900E+00	0.0000E+00	0.3501E+00	0.317100E-08	0.0000E+00	-0.107900E-10

TIME STEP NO. 20 HAS BEEN COMPLETED TOTAL ITERATION NUMBER = 0

****
* ELAPSED SIMULATION TIME = 0.1500E+09 *
****

CUMULATIVE NUMBER OF COMPUTATIONAL TIME STEPS = 30

CURRENT VALUE OF COMPUTATIONAL TIME STEP (DT) = 0.5000E+07

****
* SIMULATION RESULTS *
****

NODE	(Cw)	(Cn)	(Ca)	(Cs)	PRECIP. MASS
1	0.1000E-01	0.0000E+00	0.2500E-02	0.1000E-02	0.2893E+02
2	0.1000E-01	0.0000E+00	0.2500E-02	0.1000E-02	0.4796E+02
3	0.1000E-01	0.0000E+00	0.2500E-02	0.1000E-02	0.4796E+02
4	0.1000E-01	0.0000E+00	0.2500E-02	0.1000E-02	0.4796E+02
5	0.1000E-01	0.0000E+00	0.2500E-02	0.1000E-02	0.4797E+02
6	0.1000E-01	0.0000E+00	0.2500E-02	0.1000E-02	0.4803E+02
7	0.1000E-01	0.0000E+00	0.2500E-02	0.1000E-02	0.4904E+02
8	0.1000E-01	0.0000E+00	0.2500E-02	0.1000E-02	0.4111E+02
9	0.9553E-02	0.0000E+00	0.2388E-02	0.9553E-03	0.0000E+00
10	0.8935E-02	0.0000E+00	0.2234E-02	0.8935E-03	0.0000E+00
11	0.8150E-02	0.0000E+00	0.2037E-02	0.8150E-03	0.0000E+00
12	0.7223E-02	0.0000E+00	0.1806E-02	0.7223E-03	0.0000E+00
13	0.6201E-02	0.0000E+00	0.1550E-02	0.6201E-03	0.0000E+00
14	0.5144E-02	0.0000E+00	0.1286E-02	0.5144E-03	0.0000E+00
15	0.4112E-02	0.0000E+00	0.1028E-02	0.4112E-03	0.0000E+00
16	0.3161E-02	0.0000E+00	0.7902E-03	0.3161E-03	0.0000E+00
17	0.2330E-02	0.0000E+00	0.5825E-03	0.2330E-03	0.0000E+00
18	0.1641E-02	0.0000E+00	0.4102E-03	0.1641E-03	0.0000E+00

19	0.1095E-02	0.0000E+00	0.2738E-03	0.1095E-03	0.0000E+00
20	0.6860E-03	0.0000E+00	0.1715E-03	0.6860E-04	0.0000E+00
21	0.5127E-03	0.0000E+00	0.1282E-03	0.5127E-04	0.0000E+00

SUMMARY OF MASS BALANCE COMPUTATION FOR TRANSPORT SIMULATION

MASS BALANCE RESULTS OVER A TIME STEP

(1) NET SOLUTE MASS TRANSFERED TO PRECIP. PHASE	=	-0.1707E+00
(2) NET DECAYED SOLUTE MASS	=	0.0000E+00
(3) NET (INFLOW-OUTFLOW) SOLUTE MASS	=	-0.8129E-02
(4) NET SOLUTE MASS STORAGE CHANGES	=	0.1632E+00
(5) MASS BALANCE ERROR:	=	0.5845E-03
(6) RELATIVE MASS BALANCE ERROR:	=	0.3092E-05

CUMULATIVE MASS BALANCE RESULTS

(1) CUMULATIVE SOLUTE MASS TRANSFERED TO PRECIP. PHASE	=	-0.6242E+01
(2) CUMULATIVE DECAYED SOLUTE MASS	=	0.0000E+00
(3) CUMULATIVE (INFLOW-OUTFLOW) SOLUTE MASS	=	-0.4247E-01
(4) CUMULATIVE SOLUTE MASS STORAGE CHANGES	=	0.6203E+01
(5) CUMULATIVE MASS BALANCE ERROR	=	0.4064E-02
(6) CUMULATIVE RELATIVE MASS BALANCE ERROR	=	0.2083E-04

****
* ELEMENTAL SATURATION AND VELOCITIES *
****

ELEM.	SAT. (PH. 1)	SAT. (PH. 2)	SAT. (PH. 3)	VELOC.(PH. 1)	VELOC.(PH. 2)	VELOC.(PH. 3)
1	0.200800E+00	0.1683E+00	0.6309E+00	0.317100E-08	0.7522E-17	0.135000E-13
2	0.200800E+00	0.1683E+00	0.6309E+00	0.317100E-08	0.3146E-16	0.128400E-13
3	0.200800E+00	0.1683E+00	0.6309E+00	0.317100E-08	0.9095E-16	0.127100E-13
4	0.200800E+00	0.1683E+00	0.6309E+00	0.317100E-08	0.2171E-15	0.115100E-13
5	0.200800E+00	0.1684E+00	0.6308E+00	0.317100E-08	0.4436E-15	0.108500E-13
6	0.200800E+00	0.1699E+00	0.6292E+00	0.317100E-08	0.0000E+00	0.101800E-13
7	0.209400E+00	0.1312E+00	0.6594E+00	0.317100E-08	0.0000E+00	0.951800E-14
8	0.209400E+00	0.4552E-03	0.7451E+00	0.317100E-08	0.0000E+00	0.885800E-14
9	0.200800E+00	0.0000E+00	0.7992E+00	0.317100E-08	0.0000E+00	0.819200E-14
10	0.200800E+00	0.0000E+00	0.7992E+00	0.317100E-08	0.0000E+00	0.752700E-14
11	0.200800E+00	0.0000E+00	0.7992E+00	0.317100E-08	0.0000E+00	0.686300E-14
12	0.200800E+00	0.0000E+00	0.7992E+00	0.317100E-08	0.0000E+00	0.618900E-14
13	0.200800E+00	0.0000E+00	0.7992E+00	0.317100E-08	0.0000E+00	0.553300E-14
14	0.200800E+00	0.0000E+00	0.7992E+00	0.317100E-08	0.0000E+00	0.486800E-14
15	0.200800E+00	0.0000E+00	0.7992E+00	0.317100E-08	0.0000E+00	0.420300E-14
16	0.200800E+00	0.0000E+00	0.7992E+00	0.317100E-08	0.0000E+00	0.353700E-14
17	0.200800E+00	0.0000E+00	0.7992E+00	0.317100E-08	0.0000E+00	0.287100E-14
18	0.201000E+00	0.0000E+00	0.7990E+00	0.317100E-08	0.0000E+00	0.220500E-14
19	0.250600E+00	0.0000E+00	0.7494E+00	0.317100E-08	0.0000E+00	0.153900E-14
20	0.649900E+00	0.0000E+00	0.3501E+00	0.317100E-08	0.0000E+00	-0.107900E-10

TIME STEP NO. 30 HAS BEEN COMPLETED TOTAL ITERATION NUMBER = 0

****
* ELAPSED SIMULATION TIME = 0.2000E+09 *
****

CUMULATIVE NUMBER OF COMPUTATIONAL TIME STEPS = 40

CURRENT VALUE OF COMPUTATIONAL TIME STEP (DT) = 0.5000E+07

****
* SIMULATION RESULTS *
****

NODE	(Cw)	(Cn)	(Ca)	(Cs)	PRECIP. MASS
1	0.1000E-01	0.0000E+00	0.2500E-02	0.1000E-02	0.2259E+02
2	0.1000E-01	0.0000E+00	0.2500E-02	0.1000E-02	0.4796E+02
3	0.1000E-01	0.0000E+00	0.2500E-02	0.1000E-02	0.4796E+02
4	0.1000E-01	0.0000E+00	0.2500E-02	0.1000E-02	0.4796E+02
5	0.1000E-01	0.0000E+00	0.2500E-02	0.1000E-02	0.4797E+02
6	0.1000E-01	0.0000E+00	0.2500E-02	0.1000E-02	0.4803E+02
7	0.1000E-01	0.0000E+00	0.2500E-02	0.1000E-02	0.4904E+02
8	0.1000E-01	0.0000E+00	0.2500E-02	0.1000E-02	0.4092E+02
9	0.9715E-02	0.0000E+00	0.2429E-02	0.9715E-03	0.0000E+00
10	0.9314E-02	0.0000E+00	0.2329E-02	0.9314E-03	0.0000E+00
11	0.8788E-02	0.0000E+00	0.2197E-02	0.8788E-03	0.0000E+00
12	0.8138E-02	0.0000E+00	0.2035E-02	0.8138E-03	0.0000E+00
13	0.7381E-02	0.0000E+00	0.1845E-02	0.7381E-03	0.0000E+00
14	0.6543E-02	0.0000E+00	0.1636E-02	0.6543E-03	0.0000E+00
15	0.5657E-02	0.0000E+00	0.1414E-02	0.5657E-03	0.0000E+00
16	0.4762E-02	0.0000E+00	0.1190E-02	0.4762E-03	0.0000E+00
17	0.3896E-02	0.0000E+00	0.9739E-03	0.3896E-03	0.0000E+00
18	0.3092E-02	0.0000E+00	0.7730E-03	0.3092E-03	0.0000E+00
19	0.2379E-02	0.0000E+00	0.5948E-03	0.2379E-03	0.0000E+00
20	0.1791E-02	0.0000E+00	0.4477E-03	0.1791E-03	0.0000E+00
21	0.1528E-02	0.0000E+00	0.3819E-03	0.1528E-03	0.0000E+00

SUMMARY OF MASS BALANCE COMPUTATION FOR TRANSPORT SIMULATION

MASS BALANCE RESULTS OVER A TIME STEP

(1) NET SOLUTE MASS TRANSFERED TO PRECIP. PHASE = -0.1663E+00
(2) NET DECAYED SOLUTE MASS = 0.0000E+00
(3) NET (INFLOW-OUTFLOW) SOLUTE MASS = -0.2422E-01
(4) NET SOLUTE MASS STORAGE CHANGES = 0.1430E+00
(5) MASS BALANCE ERROR: = 0.9476E-03
(6) RELATIVE MASS BALANCE ERROR: = 0.5013E-05

CUMULATIVE MASS BALANCE RESULTS

(1) CUMULATIVE SOLUTE MASS TRANSFERED TO PRECIP. PHASE = -0.7922E+01
(2) CUMULATIVE DECAYED SOLUTE MASS = 0.0000E+00
(3) CUMULATIVE (INFLOW-OUTFLOW) SOLUTE MASS = -0.2064E+00
(4) CUMULATIVE SOLUTE MASS STORAGE CHANGES = 0.7728E+01
(5) CUMULATIVE MASS BALANCE ERROR = 0.1211E-01
(6) CUMULATIVE RELATIVE MASS BALANCE ERROR = 0.6153E-04

****
* ELEMENTAL SATURATION AND VELOCITIES *
****

ELEM.	SAT. (PH. 1)	SAT. (PH. 2)	SAT. (PH. 3)	VELOC.(PH. 1)	VELOC.(PH. 2)	VELOC.(PH. 3)
1	0.200800E+00	0.1683E+00	0.6309E+00	0.317100E-08	0.7522E-17	0.135000E-13
2	0.200800E+00	0.1683E+00	0.6309E+00	0.317100E-08	0.3146E-16	0.128400E-13
3	0.200800E+00	0.1683E+00	0.6309E+00	0.317100E-08	0.9095E-16	0.127100E-13
4	0.200800E+00	0.1683E+00	0.6309E+00	0.317100E-08	0.2171E-15	0.115100E-13
5	0.200800E+00	0.1684E+00	0.6308E+00	0.317100E-08	0.4436E-15	0.108500E-13
6	0.200800E+00	0.1699E+00	0.6292E+00	0.317100E-08	0.0000E+00	0.101800E-13
7	0.209400E+00	0.1312E+00	0.6594E+00	0.317100E-08	0.0000E+00	0.951800E-14
8	0.209400E+00	0.4552E-03	0.7451E+00	0.317100E-08	0.0000E+00	0.885800E-14
9	0.200800E+00	0.0000E+00	0.7992E+00	0.317100E-08	0.0000E+00	0.819200E-14
10	0.200800E+00	0.0000E+00	0.7992E+00	0.317100E-08	0.0000E+00	0.752700E-14
11	0.200800E+00	0.0000E+00	0.7992E+00	0.317100E-08	0.0000E+00	0.686300E-14
12	0.200800E+00	0.0000E+00	0.7992E+00	0.317100E-08	0.0000E+00	0.618900E-14
13	0.200800E+00	0.0000E+00	0.7992E+00	0.317100E-08	0.0000E+00	0.553300E-14
14	0.200800E+00	0.0000E+00	0.7992E+00	0.317100E-08	0.0000E+00	0.486800E-14
15	0.200800E+00	0.0000E+00	0.7992E+00	0.317100E-08	0.0000E+00	0.420300E-14
16	0.200800E+00	0.0000E+00	0.7992E+00	0.317100E-08	0.0000E+00	0.353700E-14
17	0.200800E+00	0.0000E+00	0.7992E+00	0.317100E-08	0.0000E+00	0.287100E-14
18	0.201000E+00	0.0000E+00	0.7990E+00	0.317100E-08	0.0000E+00	0.220500E-14
19	0.250600E+00	0.0000E+00	0.7494E+00	0.317100E-08	0.0000E+00	0.153900E-14
20	0.649900E+00	0.0000E+00	0.3501E+00	0.317100E-08	0.0000E+00	-0.107900E-10

TIME STEP NO. 40 HAS BEEN COMPLETED TOTAL ITERATION NUMBER = 0

*** OBSERVATION NODE INFORMATION ***

NODAL VALUES OF DEPENDENT VARIABLE OVER TIME

OBSERVED NODE NUMBER: 1

TIME	(Cw)	TIME	(Cw)	TIME	(Cw)
0.5000E+07	0.1000E-01	0.1000E+08	0.1000E-01	0.1500E+08	0.1000E-01
0.2000E+08	0.1000E-01	0.2500E+08	0.1000E-01	0.3000E+08	0.1000E-01
0.3500E+08	0.1000E-01	0.4000E+08	0.1000E-01	0.4500E+08	0.1000E-01
0.5000E+08	0.1000E-01	0.5500E+08	0.1000E-01	0.6000E+08	0.1000E-01
0.6500E+08	0.1000E-01	0.7000E+08	0.1000E-01	0.7500E+08	0.1000E-01
0.8000E+08	0.1000E-01	0.8500E+08	0.1000E-01	0.9000E+08	0.1000E-01
0.9500E+08	0.1000E-01	0.1000E+09	0.1000E-01	0.1050E+09	0.1000E-01
0.1100E+09	0.1000E-01	0.1150E+09	0.1000E-01	0.1200E+09	0.1000E-01
0.1250E+09	0.1000E-01	0.1300E+09	0.1000E-01	0.1350E+09	0.1000E-01
0.1400E+09	0.1000E-01	0.1450E+09	0.1000E-01	0.1500E+09	0.1000E-01
0.1550E+09	0.1000E-01	0.1600E+09	0.1000E-01	0.1650E+09	0.1000E-01
0.1700E+09	0.1000E-01	0.1750E+09	0.1000E-01	0.1800E+09	0.1000E-01
0.1850E+09	0.1000E-01	0.1900E+09	0.1000E-01	0.1950E+09	0.1000E-01
0.2000E+09	0.1000E-01				

OBSERVED NODE NUMBER: 10

TIME	(Cw)	TIME	(Cw)	TIME	(Cw)
0.5000E+07	0.5456E-03	0.1000E+08	0.1503E-02	0.1500E+08	0.2681E-02
0.2000E+08	0.3576E-02	0.2500E+08	0.4303E-02	0.3000E+08	0.4896E-02
0.3500E+08	0.5390E-02	0.4000E+08	0.5808E-02	0.4500E+08	0.6167E-02
0.5000E+08	0.6477E-02	0.5500E+08	0.6749E-02	0.6000E+08	0.6989E-02
0.6500E+08	0.7202E-02	0.7000E+08	0.7393E-02	0.7500E+08	0.7564E-02
0.8000E+08	0.7719E-02	0.8500E+08	0.7859E-02	0.9000E+08	0.7988E-02
0.9500E+08	0.8105E-02	0.1000E+09	0.8212E-02	0.1050E+09	0.8311E-02
0.1100E+09	0.8402E-02	0.1150E+09	0.8487E-02	0.1200E+09	0.8565E-02
0.1250E+09	0.8638E-02	0.1300E+09	0.8706E-02	0.1350E+09	0.8769E-02
0.1400E+09	0.8828E-02	0.1450E+09	0.8884E-02	0.1500E+09	0.8935E-02
0.1550E+09	0.8984E-02	0.1600E+09	0.9030E-02	0.1650E+09	0.9073E-02

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0.1700E+09      0.9114E-02      0.1750E+09      0.9152E-02      0.1800E+09      0.9188E-02
0.1850E+09      0.9222E-02      0.1900E+09      0.9255E-02      0.1950E+09      0.9285E-02
0.2000E+09      0.9314E-02

            ***** SAMFT1D HAS SOLVED THE PROBLEM *****


      ************************************
      *** CPU TIME USED: 28.68    SECS. ***
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