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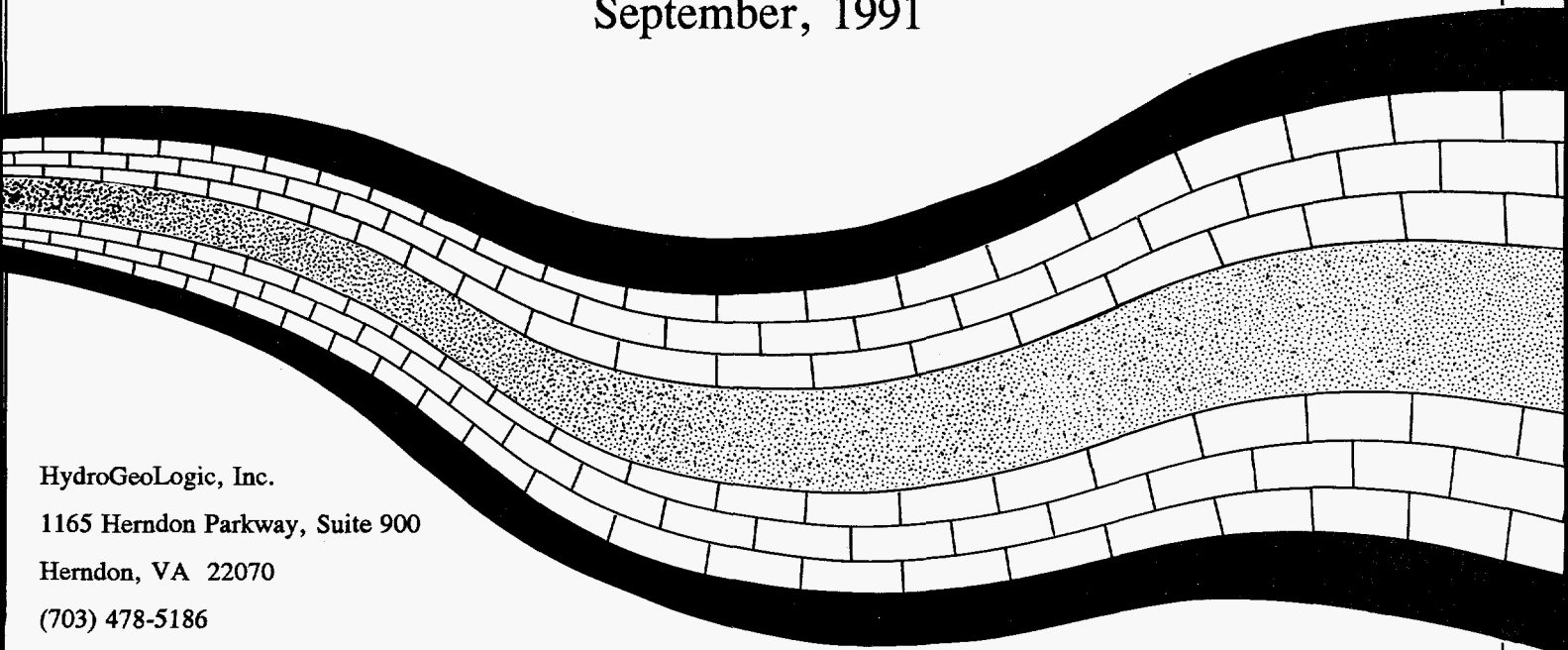
SAMFT2D

Single-phase and Multiphase Flow and Transport
in 2 Dimensions

Version 2.0

DOCUMENTATION AND USER'S GUIDE

September, 1991

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ABSTRACT

This report documents a two-dimensional finite element model, SAMFT2D, developed to simulate single-phase and multiphase fluid flow and solute transport in variably saturated porous media. The formulations 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. A fully implicit time-stepping 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 conventional 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 the Galerkin schemes with upstream weighting of phase mobilities to simulate two- or three-phase flow problems, and treat different boundary conditions in terms of source/sink terms fully implicitly. The multiphase solute transport modules employ the upstream-weighted residual schemes to handle single-species transport in multiphase fluid systems. Several example problems are presented to verify the code and to demonstrate its utility. These 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.

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1 INTRODUCTION

1.1 PURPOSE OF THE CODE

SAMFT2D is a two-dimensional, finite element code that simulates fluid flow and solute transport in variably and fully saturated porous media. The code is intended to handle single-phase, and two-phase and three-phase flow conditions using two integrated sets of computational modules. The single-phase computational modules are designed to handle situations involving flow of water (aqueous phase) and single-species transport of dissolved contaminants. Both flow and transport simulations can be performed concurrently or sequentially. Material heterogeneities and anisotropy are handled by taking full advantage of the finite element approach. Efficient matrix computational and solution schemes are employed in conjunction with linear rectangular elements to analyze problems involving highly nonlinear soil moisture characteristics. Several types of boundary conditions can be accommodated including prescribed pressure head and flux conditions, water-table conditions, recharge, infiltration, and sinks and sources.

The multiphase flow modules are coded using fully implicit Galerkin finite element techniques with storage matrix lumping and upstream weighting of phase mobilities. These modules are designed to handle situations involving (1) two-phase flow of water and NAPL (NonAqueous Phase Liquid) in the two-phase fluid system, (2) three-phase flow of water, NAPL and air (vapor phase), and (3) two-phase flow of water and NAPL in the three-phase fluid system. The multiphase solute transport modules use the upstream-weighted residual finite element scheme and are designed to simulate single-species contaminant transport taking into

account the maximum solubility constraint for the component. Several types of boundary conditions commonly encountered in field investigations of NAPL contamination problems can be handled by the code. Both fluid flow and solute transport simulations in the SAMFT2D code can be handled concurrently or sequentially.

1.2 OVERVIEW OF CODE CAPABILITIES AND SALIENT FEATURES

Multi-dimensional 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 a wide range of field conditions. Recognizing this point, SAMFT2D 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. SAMFT2D can perform transient analyses (whenever practical) or 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, either 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 these problems concurrently or sequentially in a single computer run.

2. The finite element formulation and nonlinear solution procedures in SAMFT2D are based on state-of-the-art technology designed to accommodate a wide range of field conditions including highly nonlinear moisture characteristics, material heterogeneity and anisotropy, and rapidly fluctuating transient flow boundary conditions.

3. The flow simulator of SAMFT2D can handle various boundary conditions and

physical processes including infiltration, evaporation, well pumping and recharging, and varying 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 SAMFT2D is designed to have upstream weighting capability to circumvent numerical oscillations. The scheme can accommodate first-order decay as well as linear equilibrium sorption. Both pulse and step releases of contaminants can be simulated. Additionally, the solubility limit of the contaminant component can be incorporated in a multiphase transport simulation and mass balance calculation. These capabilities make it advantageous to use SAMFT2D in the prediction of fate and transport of miscible and immiscible contaminants with dissolved constituents.

1.3 APPLICABILITY OF THE CODE

The SAMFT2D code has many practical applications. Typical examples include the following:

- Investigation of moisture movement and air flow in variably saturated subsurface systems
- Investigation of immiscible flow of Dense and Light NonAqueous Phase Liquids (DNAPL and LNAPL) and miscible transport of dissolved constituents or components in the unsaturated and saturated zones of the subsurface system
- Investigation of groundwater flow in confined and unconfined aquifer systems
- Investigation of transport of dissolved contaminants in the subsurface soil or groundwater system
- Investigation of leachate migration from land disposal units

- Investigation of potential for migration of radionuclides or mixed wastes from subsurface repositories or buried canisters.

1.4 CODE USER REQUIREMENTS

In order to apply the SAMFT2D code effectively, the user will need:

- a thorough understanding of hydrogeological principles
- a basic understanding of numerical modeling 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

SAMFT2D 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 personal computers 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 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 a 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 SAMFT2D perform two-dimensional finite element simulations of water flow and solute transport in variably saturated and fully saturated porous media. These modules employ state-of-the-art numerical techniques 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 hazardous 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 anisotropy and heterogeneity of permeability. For solute transport simulations, SAMFT2D accounts for advection, hydrodynamic dispersion, equilibrium sorption, and first-order decay.

The multiphase modules of SAMFT2D perform two-phase and three-phase flow and single-species transport simulations. The fluids considered include water, NAPL (NonAqueous Phase Liquid) contaminant, and air or vapor. For multiphase transport simulations, SAMFT2D accounts for solute partitioning among various fluid phases and the porous matrix as well as precipitation of the component.

The user is permitted to employ the following coordinate systems:

- two-dimensional Cartesian coordinates (x,y) in a horizontal plane
- two-dimensional Cartesian coordinates (x,y) in a vertical plane with the y-axis pointing vertically upward.

2.2 GOVERNING AND SUPPLEMENTARY EQUATIONS FOR SINGLE-PHASE MODELS

The single-phase components of SAMFT2D are formulated based upon two governing equations, one describing flow of water (aqueous-phase) and the other describing single-species solute transport. These 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 SAMFT2D code uses gauge pressure head of water (the aqueous phase) as the primary dependent variable. The governing equation for water flow in a variably saturated porous medium may be expressed in the form:

$$\frac{\partial}{\partial x_i} \left[\rho_w K_{ij} k_{rw} \left(\frac{\partial \psi}{\partial x_j} + e_j \right) \right] = \frac{\partial}{\partial t} (\rho_w \phi S_w) - \rho_w q \quad (2.1)$$

where ρ_w is the density of water, ψ is the gauge, water-pressure head, K_{ij} is the saturated hydraulic conductivity tensor, k_{rw} is the relative permeability with respect to the water phase, x_i ($i = 1, 2$) are spatial coordinates, t is time, e_j is the unit vector assumed to be vertically upward, S_w is water-phase saturation, ϕ is the effective porosity, and q is the volumetric flow rate via sources (or sinks) per unit volume of the porous medium.

Note that ψ and K_{ij} are defined as

$$\psi = (p_w - p_{atm}) / \rho_w g \quad (2.2a)$$

and

$$K_{ij} = k_{ij} \rho_w g / \mu_w \quad (2.2b)$$

where p_w is the water-phase pressure, p_{atm} is the atmospheric pressure, g is the gravitational acceleration constant, k_{ij} is the intrinsic permeability tensor, and μ_w is the dynamic viscosity of water.

For slightly compressible fluid, equation (2.1) can be written in the form:

$$\frac{\partial}{\partial x_i} \left[(K_{ij} k_{rw} \frac{\partial \psi}{\partial x_j} + e_j) \right] = \eta \frac{\partial \psi}{\partial t} - q \quad (2.3)$$

where η is a coefficient defined as:

$$\eta = S_w S_s + \phi \frac{dS_w}{d\psi} \quad (2.4)$$

The coefficient S_s in equation (2.4) is known as specific storage and is defined as $S_s = \rho_w g (\phi \beta_w + \beta_s^*)$, where g is the gravitational acceleration, and β_s^* and β_w are coefficients of vertical compressibility of the porous medium formation and water, respectively.

The initial and boundary conditions of the variably saturated water flow problem are:

$$\psi(x_i, 0) = \psi_o(x_i) \quad (2.5)$$

$$\psi(x_i, t) = \bar{\psi} \text{ on } B_1 \quad (2.6)$$

and

$$V_i n_i = -V_n \text{ on } B_2 \quad (2.7)$$

where ψ_0 is the initial head value, B_1 is the portion of the flow boundary where $\bar{\psi}$ is prescribed as ψ , V_i is the Darcy velocity vector, B_2 is the portion of the flow boundary where the outward normal velocity is prescribed as $-V_n$, and n_i is the outward unit normal vector. Note that V_n is considered positive for inward flux, and negative for outward flux.

In order to solve the variably saturated flow 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 (Brooks and Corey, 1966; van Genuchten, 1976):

$$k_{rw} = S_e^n \quad (2.8a)$$

and

$$k_{rw} = S_e^{1/2} [1 - (1 - S_e^{1/\gamma})^\gamma]^2 \quad (2.8b)$$

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):

$$\frac{S_w - S_{wr}}{1 - S_{wr}} = \begin{cases} \frac{1}{[1 + (\alpha |\psi - \psi_a|)^\beta]^\gamma} & \text{for } \psi < \psi_a \\ 1 & \text{for } \psi \geq \psi_a \end{cases} \quad (2.9)$$

where α and β are empirical parameters, ψ_a is the air entry pressure head value, and S_{wr} is the residual water saturation. The parameters β and γ are usually related by $\gamma = 1-1/\beta$.

Equation (2.3) is solved numerically using the Galerkin finite element method subject to the initial and boundary conditions given in (2.5) through (2.7). After the distributions of ψ and S_w have been determined, Darcy velocity components are calculated from:

$$V_i = -K_{ij} k_{rw} \left(\frac{\partial \psi}{\partial x_j} + e_j \right) \quad (2.10)$$

2.2.2 Solute Transport with Single-Phase Flow

The governing equation for transport of a non-conservative single component in a variably saturated porous medium takes the form:

$$\begin{aligned} \frac{\partial}{\partial x_i} (D_{ij} \frac{\partial c}{\partial x_j}) - \frac{\partial}{\partial x_i} (V_i c) &= \frac{\partial}{\partial t} [\phi S_w c + \rho_s (1-\phi) c_s] - q c^* \\ &+ \lambda [\phi S_w c + \rho_s (1-\phi) c_s] \end{aligned} \quad (2.11)$$

where D_{ij} is the apparent hydrodynamic dispersion tensor, c is solute concentration in the fluid, V_i is the Darcy velocity, ϕ is the effective porosity, ρ_s is the density of solid grains, c_s is the adsorbed concentration, λ is the first-order decay coefficient, and c^* is the solute concentration

in the injected fluid.

Assuming that the relation between adsorbed and dissolved concentration is described by a linear equilibrium isotherm, equation (2.11) can be expressed as

$$\begin{aligned} \frac{\partial}{\partial x_i} (D_{ij} \frac{\partial c}{\partial x_j}) - \frac{\partial}{\partial x_i} (V_i c) = \frac{\partial}{\partial t} \left[\phi S_w \left(1 + \frac{\rho_s(1-\phi)k_d}{\phi S_w} \right) c \right] - qc^* \\ + \lambda \phi S_w \left[1 + \frac{\rho_s(1-\phi)k_d}{\phi S_w} \right] c \end{aligned} \quad (2.12)$$

where k_d is the distribution coefficient.

Equation (2.12) reduces to

$$\frac{\partial}{\partial x_i} (D_{ij} \frac{\partial c}{\partial x_j}) - \frac{\partial}{\partial x_i} (V_i c) = \frac{\partial}{\partial t} (\phi S_w R c) + \lambda \phi S_w R c - q c^* \quad (2.13)$$

where R is the retardation factor defined as

$$R = 1 + \frac{\rho_s(1-\phi)k_d}{\phi S_w} = 1 + \frac{\rho_B k_d}{\phi S_w} \quad (2.14)$$

with the bulk density ρ_B being defined as $(1-\phi)\rho_s$. Expanding the convective and mass accumulation terms of equation (2.13) and using the continuity equation of fluid flow, one obtains

$$\begin{aligned} \frac{\partial}{\partial x_i} (D_{ij} \frac{\partial c}{\partial x_j}) - V_i \frac{\partial c}{\partial x_i} = \phi S_w R \frac{\partial c}{\partial t} + c \frac{\partial}{\partial t} (\phi S_w) + c \frac{\partial}{\partial t} (\rho_B k_d) \\ - c \frac{\partial}{\partial t} (\phi S_w) + q(c-c^*) + \lambda \phi S_w R c \end{aligned} \quad (2.15)$$

which, assuming that the time derivative of $(\rho_B k_d)$ is negligible, reduces to

$$\frac{\partial}{\partial x_i} (D_{ij} \frac{\partial c}{\partial x_j}) - V_i \frac{\partial c}{\partial x_i} = \phi S_w R (\frac{\partial c}{\partial t} + \lambda c) + q(c - c^*) \quad (2.16)$$

Note that the term $q(c - c^*)$ is zero in the case where q corresponds to the specific discharge of a pumped well, because $c \equiv c^*$. The hydrodynamic dispersion tensorial components are computed using the following constitutive relations (Scheidegger, 1961):

$$D_{11} = \frac{\alpha_L (V_1)^2}{|V|} + \frac{\alpha_T (V_2)^2}{|V|} + D_w^* \quad (2.17a)$$

$$D_{22} = \frac{\alpha_L (V_2)^2}{|V|} + \frac{\alpha_T (V_1)^2}{|V|} + D_w^* \quad (2.17b)$$

$$D_{12} = D_{21} = (\alpha_L - \alpha_T) \frac{V_1 V_2}{|V|} \quad (2.17c)$$

where α_L and α_T are longitudinal and transverse dispersivities, respectively, and D_w^* is the apparent molecular diffusion in the water-phase of the porous medium:

The apparent molecular diffusion coefficient of the water-phase is computed by the code using the following relation:

$$D_w^* = (\tau \phi S_w^n) D_{mw} \quad (2.18)$$

where τ is a tortuosity factor, D_{mw} is the free-water molecular diffusion coefficient, and n is an exponent parameter. Note that equation (2.18) corresponds to the Millington-Quirk equation if τ and n are set equal to $\phi^{1/3}$ and $10/3$, respectively.

Equation (2.16) is the required form of the transport equation and will be approximated using the upstream weighted residual finite element technique of Huyakorn and Nilkuha (1979). The initial and boundary conditions associated with equation (2.16) are as follows:

$$c(x_1, x_2, 0) = c_o \quad (2.19)$$

$$c(x_1, x_2, t) = \bar{c} \text{ on } B'_1 \quad (2.20a)$$

$$D_{ij} \frac{\partial c}{\partial x_j} n_i = q_c^D \text{ on } B'_2 \quad (2.20b)$$

$$D_{ij} \frac{\partial c}{\partial x_j} n_i - V_i n_i c = q_c^T \text{ on } B'_3 \quad (2.20c)$$

where B'_1 is the portion of the boundary where concentration is prescribed as \bar{c} , and B'_2 and B'_3 are portions of the boundary where the dispersive and the total solute mass fluxes are prescribed as q_c^D and q_c^T , respectively.

2.3 GOVERNING AND SUPPLEMENTARY EQUATIONS FOR MULTIPHASE MODELS

The multiphase components of SAMFT2D are formulated based upon immiscible flow equations (one equation for each active fluid 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 Equations

We consider a general situation involving flow of three active fluid phases: water, NAPL (Nonaqueous Phase Liquid), and air or vapor. A straight forward simplification of the formulation presented can be made for cases involving only two active phases. The governing equations for three-phase flow may be expressed as

$$\frac{\partial}{\partial x_i} \left[k_{ij} \tau_\ell \frac{\partial \Phi_\ell}{\partial x_j} \right] = \frac{\partial}{\partial t} (\theta \rho_\ell S_\ell) - \dot{M}_\ell, \quad \ell = w, n, a \quad (2.21)$$

where subscript ℓ refers to the three fluid phases: water (w), NAPL (n) and air (a), k_{ij} is the intrinsic permeability tensor, τ_ℓ and Φ_ℓ are the mobility and fluid potential of phase ℓ , respectively, θ , ρ_ℓ and S_ℓ are porosity, fluid density and phase saturation, \dot{M}_ℓ is the mass flow rate of phase ℓ via sources or sinks per unit volume of the porous medium.

The phase mobility and fluid potential are defined as

$$\tau_\ell = k_{r\ell} \rho_\ell / \mu_\ell \quad (2.22)$$

and

$$\frac{\partial \Phi_\ell}{\partial x_j} = \frac{\partial p_\ell}{\partial x_j} + \rho_\ell g \frac{\partial Z}{\partial x_j} \quad (2.23)$$

where $k_{r\ell}$ is the relative permeability, μ_ℓ is the dynamic viscosity, and Z is the elevation above a given datum.

The initial and boundary conditions of the multiphase flow problem may be represented by

$$p_\ell(x_i, 0) = p_\ell^o(x_i) \quad (2.24)$$

$$p_\ell(x_i, t) = \tilde{p}_\ell \text{ on } B_1 \quad (2.25a)$$

and

$$V_{i\ell} n_i = -\tilde{V}_\ell \text{ on } B_2 \quad (2.25b)$$

where p_ℓ^o is the initial phase pressure value, B_1 is the portion of the flow boundary where p_ℓ is prescribed as \tilde{p}_ℓ , $V_{i\ell}$ is the Darcy velocity vector for phase ℓ , B_2 is the boundary portion where the outward normal velocity of phase ℓ is prescribed as $-\tilde{V}_\ell$, and n_i is the outward unit normal vector.

In addition to the three governing equations, there are supplementary equations given by:

$$S_w + S_n + S_a = 1 \quad (2.26a)$$

$$p_n - p_w = \bar{P}_{cnw}(S_w) \quad (2.26b)$$

$$p_a - p_n = \bar{P}_{can}(S_w, S_n) \quad (2.26c)$$

$$p_a - p_w = \bar{P}_{can} + \bar{P}_{cnw} \quad (2.26d)$$

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

$$\bar{P}_{cnw} = \hat{\alpha} P_{cnw}(S_w) + (1-\hat{\alpha}) P_{cnw}(S_w=1) \quad (2.27a)$$

$$\bar{P}_{can} = \hat{\alpha} P_{can}(S_a) + (1-\hat{\alpha}) [P_{caw}(S_a) - P_{cnw}(S_w=1)] \quad (2.27b)$$

with either $0 \leq \hat{\alpha} = \min(1, S_n/S_n^*)$ and S_n^* being critical NAPL saturation.

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 unknown variables are: p_w , p_n , p_a , S_w , S_n and S_a . They can be determined using equations (2.21), (2.26a), (2.26b) and (2.26c).

In a three-phase flow situation, we select p_n , S_n and S_w as the first, second and third primary variables, respectively. In terms of these primary variables, the remaining three variables may be expressed as:

$$S_a = 1 - S_w - S_n \quad (2.28a)$$

$$P_w = P_n - \bar{P}_{cnw}(S_w) \quad (2.28b)$$

and

$$P_a = P_w + \bar{P}_{cnw}(S_w) + \bar{P}_{can}(S_a) \quad (2.28c)$$

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,

$$P_{cnw} = P_{cnw}(S_w) \quad (2.29a)$$

and

$$P_{can} = P_{can}(S_a) \quad (2.29b)$$

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

$$P_{caw} = P_{caw}(S_a) \quad (2.29c)$$

The phase pressure relations including smooth transition of two phases (water-air) to three phases (water-NAPL-air) during simulations are described by equations (2.27a) and (2.27b).

(b) Relative Permeability

The three-phase relative permeability functions used are:

Relative permeability to water phase,

$$k_{rw} = k_{rw}^{wn}(S_w) \quad (2.30a)$$

relative permeability to air phase,

$$k_{ra} = k_{ra}^{na}(S_a) \quad (2.30b)$$

and relative permeability to NAPL phase,

$$k_{rn} = k_{rn}(S_w, S_n) \quad (2.30c)$$

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

$$k_{rn}(S_w, S_a) = k_{rn}^{*wn} \left[(k_{rn}^{wn}/k_{rn}^{*wn} + k_{rw}) (k_{rn}^{na}/k_{rn}^{*wn} + k_{ra}) - (k_{rw} + k_{ra}) \right] \quad (2.31a)$$

with the constraint

$$k_{rn} \geq 0 \quad (2.31b)$$

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

(c) Functional Relations of Capillary Pressure and Relative Permeability

The SAMFT2D code also provides the user with an additional option of using functional

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

$$\tilde{S} = [1 + (\alpha \tilde{h})^\beta]^{-\gamma} \quad (2.32)$$

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 (2.32) may be rearranged to give

$$\tilde{h} = \frac{1}{\alpha} [(1/\tilde{S})^{1/\gamma} - 1]^{1/\beta} \quad (2.33)$$

For the three-phase (w-n-a) system, equation (2.33) 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:

$$P_{cnw} = \frac{\sigma_{nw} \rho_{fw} g}{\alpha \sigma_{aw}} \left[(\bar{S}_w)^{-1/\gamma} - 1 \right]^{1/\beta} \quad (2.34a)$$

$$P_{can} = \frac{\sigma_{an} \rho_{fw} g}{\alpha \sigma_{aw}} \left[(1 - \bar{S}_a)^{-1/\gamma} - 1 \right]^{1/\beta} \quad (2.34b)$$

and

$$P_{caw} = \frac{\rho_{fw} g}{\alpha} \left[(1 - \bar{S}_a)^{-1/\gamma} - 1 \right]^{1/\beta} \quad (2.34c)$$

where

$$\bar{S}_w = \frac{S_w - S_{wr}}{1 - S_{wr}} \quad (2.35a)$$

and

$$\bar{S}_a = \frac{S_a}{1 - S_{wr}} \quad (2.35b)$$

In equations (2.34a) - (2.34c), 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 (2.34a) - (2.34c) need to be used in conjunction with the pressure relations given in equations (2.27a) - (2.27b) 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:

$$k_{rw} = (\bar{S}_w)^{1/2} \left\{ 1 - \left[1 - (\bar{S}_w)^{1/\gamma} \right]^\gamma \right\}^2 \quad (2.36a)$$

$$k_{rn} = (\bar{S}_n - \bar{S}_{nr})^{1/2} \left\{ \left[1 - (\bar{S}_w)^{1/\gamma} \right]^\gamma - \left[1 - (\bar{S}_L)^{1/\gamma} \right]^\gamma \right\}^2 \quad (2.36b)$$

and

$$k_{ra} = (\bar{S}_a)^{1/2} [1 - (\bar{S}_L)^{1/\gamma}]^{2\gamma} \quad (2.36c)$$

where

$$\bar{S}_n = \frac{S_n}{1 - S_{wr}} \quad (2.37a)$$

$$\bar{S}_L = \bar{S}_n + \bar{S}_w \quad (2.37b)$$

and

$$\bar{S}_{nr} = \frac{S_{nr}}{1 - S_{wr}} \quad (2.37c)$$

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:

$$k_{rw} = k_{rw}^{wn} (\bar{S}_w) = (\bar{S}_w)^{N+2} \quad (2.38a)$$

$$k_{rn} = (\bar{S}_n - \bar{S}_{nr})^2 [(\bar{S}_L)^N - (\bar{S}_w)^N] \quad (2.38b)$$

and

$$k_{ra} = k_{ra}^{na} (\bar{S}_a) = (\bar{S}_a)^2 [1 - (\bar{S}_L)^N] \quad (2.38c)$$

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 correspond to equations (2.29a) - (2.29c). The relative permeability functions are represented by equations (2.31) and (2.32) for tabulated data and by either pair of equations (2.36a) and (2.36c), or (2.38a) and (2.38c) 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:

$$\rho_w = \rho_w^o e^{\beta_w(p_w - p^*)} \approx \rho_w^o [1 + \beta_w (p_w - p^*)] \quad (2.39a)$$

$$\rho_n = \rho_n^o e^{\beta_n(p_n - p^*)} \approx \rho_n^o [1 + \beta_n (p_n - p^*)] \quad (2.39b)$$

$$\rho_a = \frac{p_a M}{RT} = \beta_a p_a \quad (2.39c)$$

and porosity is described by,

$$\theta = \phi(P_w) \approx \theta_o [1 + \beta_s (p_w - p^*)] \quad (2.40)$$

where

$$\begin{aligned}
p_o &= \text{reference pressure} \\
\rho_w^o &= \text{water density at } p_w = p^* \\
\rho_n^o &= \text{NAPL density at } p_n = p^* \\
\beta_w &= \frac{1}{\rho_w} \left. \frac{\partial \rho_w}{\partial p_w} \right|_T, \text{ water compressibility} \\
\beta_n &= \frac{1}{\rho_n} \left. \frac{\partial \rho_n}{\partial p_n} \right|_T, \text{ NAPL compressibility} \\
\beta_a &= \frac{M}{RT}, \text{ air compressibility factor} \\
M &= \text{Molecular weight of the gas phase} \\
R &= \text{Universal gas constant} \\
T &= \text{Constant (absolute) temperature} \\
\beta_s &= \frac{1}{\theta} \left. \frac{\partial \theta}{\partial p_w} \right|_T \text{ solid matrix compressibility} \\
\theta_o &= \text{Porosity at } p_w = p_o
\end{aligned}$$

Note that $\beta_s = \beta_s^*/\theta$, where β_s^* is the vertical compressibility of the formation introduced previously (page 2-3).

2.3.1.3 Initial and Boundary Conditions

The initial conditions needed for solving the multiphase flow equations (2-21) are:

$$p_n(x_i, 0) = p_{ni}(x, y) \quad (2.41a)$$

$$S_n(x, y, 0) = S_{ni}(x, y) \quad (2.41b)$$

$$S_w(x, y, 0) = S_{wi}(x, y) \quad (2.41c)$$

where $P_i(x,y)$, $S_{ni}(x,y)$ and $S_{wi}(x,y)$ are the initial NAPL pressure and initial NAPL and water saturations, respectively. These are generally functions of the coordinates (x,y) .

The boundary conditions for a multiphase flow problem may be expressed in terms of prescribed phase pressure or prescribed fluid flux conditions. For each mobile phase ℓ , the two types of boundary conditions are represented by:

$$p_\ell(x,y,t) = \tilde{p}_\ell \quad \text{on } B_1 \quad (2.42a)$$

and

$$\rho_\ell V_{i\ell} n_i = -\tilde{M}_\ell \quad \text{on } B_2 \quad (2.42b)$$

where \tilde{p}_ℓ and \tilde{M}_ℓ are the prescribed values of phase pressure and mass flux on boundary portions B_1 and B_2 , respectively, $V_{i\ell}$ is the Darcy velocity of phase ℓ and n_i is the outward unit normal vector. Note that \tilde{M}_ℓ is considered positive for inward flux and negative for outward flux.

2.3.2 Solute Transport with Multiphase Flow

2.3.2.1 Transport Equations

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

$$\frac{\partial}{\partial x_i} \left[D_{\ell ij} \frac{\partial}{\partial x_j} (\rho_\ell c_\ell) \right] - \frac{\partial}{\partial x_i} (V_{i\ell} \rho_\ell c_\ell) = \frac{\partial}{\partial t} (\phi S_\ell \rho_\ell c_\ell) + \lambda_\ell \phi S_\ell \rho_\ell c_\ell \quad (2.43)$$

$$+ Q_\ell \rho_\ell (c_\ell - c_\ell^*) - \Gamma_\ell$$

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, $D_{\ell ij}$ is the apparent hydrodynamic dispersion coefficient with respect to fluid phase ℓ , $V_{\ell i}$ 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. The "precipitated phase" is an immobile (liquid or solid) 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 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 (2.43) may be expressed in the form:

$$\frac{\partial}{\partial x_i} \left[D_{\ell ij} \rho_\ell \frac{\partial c_\ell}{\partial x_j} \right] - V_{\ell i} \rho_\ell \frac{\partial c_\ell}{\partial x_i} = \phi S_\ell \rho_\ell \frac{\partial c_\ell}{\partial t} + \lambda_\ell \phi S_\ell \rho_\ell c_\ell + Q_\ell \rho_\ell (c_\ell - c_\ell^*) - \Gamma_\ell \quad (2.44)$$

where the term $\frac{\partial}{\partial x_i} \left[D_{\ell ij} c_\ell \frac{\partial \rho_\ell}{\partial x_j} \right]$ has been neglected, and the following flow continuity

equation has been used:

$$-\frac{\partial}{\partial t} (V_{li} \rho_l) = \frac{\partial}{\partial t} (\phi S_l \rho_l) \quad (2.45)$$

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

$$\frac{\partial}{\partial t} (\rho_p S_p \phi) + \lambda_p S_p = \Gamma_p \quad (2.46)$$

where ρ_p and S_p are density and saturation 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

$$\frac{\partial}{\partial t} [(1 - \phi) \rho_s c_s] + \lambda_s c_s = \Gamma_s \quad (2.47)$$

where c_s and λ_s are the solute concentration and the coefficient of decay in the solid phase, respectively, and Γ_s is the rate of solute mass transfer between the soil matrix and all other phases. Equation (2.43) may be summed with respect to all fluid phases (w,n,a) and combined with (2.45) and (2.46) to give

$$\begin{aligned} \sum_l \left[\frac{\partial}{\partial x_i} \left[D_{lij} \rho_l \frac{\partial c_l}{\partial x_j} \right] - V_{li} \rho_l \frac{\partial c_l}{\partial x_i} \right] &= \sum_l (\phi S_l \rho_l \frac{\partial c_l}{\partial t} \\ &+ \lambda_l \phi S_l \rho_l c_l) + (1 - \phi) \rho_s \left[\frac{\partial c_s}{\partial t} + \lambda_s c_s \right] + \sum_l \rho_l Q_l (c_l - c_l^*) \\ &+ \frac{\partial}{\partial t} [\rho_p S_p \phi] + \lambda_p \phi \rho_p S_p \end{aligned} \quad (2.48)$$

where the following mass-conservation constraint has been applied:

$$\Gamma_w + \Gamma_n + \Gamma_a + \Gamma_s + \Gamma_p = 0 \quad (2.49)$$

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:

$$c_n = \kappa_n c_w \quad (2.50a)$$

$$c_a = \kappa_a c_w \quad (2.50b)$$

$$c_s = k_d \rho_w c_w \quad (2.50c)$$

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. 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

$$\kappa_n = \kappa_a / \kappa_a^* \quad (2.51)$$

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

Equation (2.48) can be combined with (2.50a)-(2.50c) to give the following equation:

$$\begin{aligned}
& \frac{\partial}{\partial x_i} \left[(D_{wij} \rho_w + \kappa_n \rho_n D_{nij} + \kappa_a \rho_a D_{aij}) \frac{\partial c_w}{\partial x_j} \right] \\
& - (V_{wi} \rho_w + \kappa_n \rho_n V_{ni} + \kappa_a \rho_a V_{ai}) \frac{\partial c_w}{\partial x_i} = \phi (RS_w \rho_w + \kappa_n S_n \rho_n + \kappa_a S_a \rho_a) \frac{\partial c_w}{\partial t} \\
& \quad + \phi \lambda (RS_w \rho_w + \kappa_n S_n \rho_n + \kappa_a S_a \rho_a) c_w \quad (2.52) \\
& \quad + \sum_{\ell} \rho_{\ell} Q_{\ell} (c_{\ell} - c_{\ell}^*) + \frac{\partial}{\partial t} [\rho_p \phi S_p] \\
& \quad + \lambda_p \phi \rho_p S_p
\end{aligned}$$

where R is given by

$$R = 1 + \frac{(1 - \phi) \rho_s k_d}{\phi S_w} \quad (2.53)$$

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

We now introduce the following definitions:

$$D_{Tij} = \rho_w D_{wij} + \rho_n \kappa_n D_{nij} + \rho_a \kappa_a D_{aij} \quad (2.54)$$

$$V_{Ti} = \rho_w V_{wi} + \rho_n \kappa_n V_{ni} + \rho_a \kappa_a V_{ai} \quad (2.55)$$

$$R_T = R \rho_w S_w + \kappa_n \rho_n S_n + \kappa_a \rho_a S_a \quad (2.56)$$

$$Q_T = \rho_w Q_w + \rho_n Q_n \kappa_n + \rho_a Q_a \kappa_a \quad (2.57)$$

$$(Qc)_T^* = \rho_w Q_w C_w^* + \rho_n Q_n C_n^* + \rho_a Q_a C_a^* \quad (2.58)$$

Equation (2.52) may be combined with (2.54) - (2.58) to give the following governing equation:

$$\begin{aligned} \frac{\partial}{\partial x_i} \left[D_{Tij} \frac{\partial c_w}{\partial x_j} \right] - V_{Ti} \frac{\partial c_w}{\partial x_i} = \phi R_T \left(\frac{\partial c_w}{\partial t} + \lambda c_w \right) + \\ \frac{\partial}{\partial t} [m_p] + \lambda_p m_p + Q_T c_w - (Qc)_T^* \end{aligned} \quad (2.59)$$

where $m_p = \rho_p S_p \phi$.

Equation (2.59) needs to be solved numerically subject to the following constraints:

$$c_w \leq c_{ws} \quad (2.60)$$

and

$$m_p \geq 0 \quad (2.61)$$

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

2.3.2.2 Supplementary Equations

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

$$V_{li} = - \frac{k_{ij} k_{rl}}{\mu_l} \frac{\partial \Phi_l}{\partial x_j} \quad (2.62)$$

$$D_{\ell ij} = \alpha_T |V_\ell| \delta_{ij} + (\alpha_L - \alpha_T) \frac{V_{\ell i} V_{\ell j}}{|V_\ell|} + (\phi \tau^* S_\ell^N) D_{m\ell} \delta_{ij} \quad (2.63)$$

where α_L and α_T are longitudinal and transverse dispersivities, $D_{m\ell}$ 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 $V_{\ell i} = 0$.

2.3.2.3 Initial and Boundary Conditions

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

$$c_w(x_i, 0) = c_w(x_i) \quad (2.64)$$

$$c_w(x_i, t) = \bar{c}_w \text{ on } B'_1 \quad (2.65)$$

$$\sum_{\ell} (D_{ij\ell} \frac{\partial c_{\ell}}{\partial x_j} n_i) = \dot{m}_D \text{ on } B'_2 \quad (2.65)$$

$$\sum_{\ell} (D_{ij\ell} \frac{\partial c_{\ell}}{\partial x_j} - V_{i\ell}) n_i = \dot{m}_T \text{ on } B'_3 \quad (2.65)$$

where B'_1 is the boundary portion where the solute concentration in the water phase is prescribed \bar{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 convention for \dot{m}_D and \dot{m}_T is 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 multiphase flow model of SAMFT2D 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. The medium dispersivity is assumed to correspond to that of an isotropic porous medium and hence related to two constants, α_L and α_T , which are the longitudinal and transverse dispersivities
- Adsorption and decay of the solute may be described by a linear equilibrium isotherms and first order decay constants.

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. For each fluid phase, the hydrodynamic dispersion coefficient is defined as the sum of the coefficients of mechanical dispersion and molecular diffusion. The medium dispersivity is assumed to correspond to that of an isotropic porous medium and hence related to two constants, α_L and α_T , which are the longitudinal and transverse dispersivities
- Adsorption and decay of the solute in the solid and fluid phases may be described by linear equilibrium isotherms and first order decay constants.

2.5 LIMITATIONS

The SAMFT2D code has the following limitations:

- In performing single-phase or multiphase flow analysis, the code neglects effects of temperature variation and non-Darcian flow or non-Newtonian behavior of the fluids
- The code considers only single-porosity soil or aquifer media. It does not rigorously 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 are also neglected.

2.6 INPUT DATA

Input data and parameters required by the single-phase and multiphase models of SAMFT2D are summarized below.

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 components, k_{xx} , k_{yy} and k_{xy} (L^2)
 - Volume compressibility, β_s (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, β_w (LT^2/M)
- (4) Initial and Boundary Conditions
 - Initial distribution of water-phase pressure, p_w^o ($ML^{-1} T^{-2}$)
 - Prescribed values of p_w at specified Dirichlet boundary nodes, \bar{p}_w ($ML^{-1} T^{-2}$)
 - Prescribed values of water fluxes at

specified flux nodes, q_w ($L^2 T^{-1}$)

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)
 - Transverse dispersivity, α_T (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 components, V_1 and V_2 (LT^{-1})
- (5) Water-phase saturation, S_w
- (6) Initial and boundary conditions
 - Initial distribution of concentration, c_0 (ML^{-3})
 - Prescribed values of concentration, \bar{c} (ML^{-3})
 - Prescribed values of solute flux, \bar{m} ($ML^{-1} T^{-1}$)

- (7) Boundary geometry and fluid flux data at the boundary nodes

(ML⁻¹ T⁻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. Functional or tabulated relationships are used to describe the relative permeabilities of various fluid phases and capillary behavior. A full description of data requirements is provided in Section 8.3 of Chapter 8.

2.7 OUTPUT

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 and element centroidal values of Darcy velocity components 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 and 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, SAMFT2D 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 water 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 SAMFT2D includes nodal values (at user-selected time levels) of solute concentration. SAMFT2D 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 SAMFT2D code is also capable of performing concurrent 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 a velocity backup file for the transport simulation. 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 the primary variables (pressure and saturations) at specified time levels. If required, element centroidal values of Darcy velocities and phase saturations can also be printed. 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 mass 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, SAMFT2D 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.

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 the Galerkin finite element approximation technique with upstream weighting of phase mobilities and a fully implicit Newton-Raphson scheme. The transport equations for both single and multiple 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

The governing equation for water flow (2.3) is discretized using the conventional Galerkin finite element method. In the Galerkin procedure, the pressure head function is represented by a trial function of the form

$$\psi(x_i, t) = N_J(x_i) \phi_J(t) \quad , \quad J = 1, 2, \dots, n \quad (3.1)$$

where $N_J(x_i)$ and $\phi_J(t)$ are basis functions and nodal values of pressure head at time t , respectively, n is the number of nodes in the finite element network, and repeated indices imply

nodal summation. Applying the Galerkin criterion to (2.3) and transforming the second-order derivative term, one obtains

$$\begin{aligned}
 & \int_R K_{ij} k_{rw} \frac{\partial N_i}{\partial x_i} \frac{\partial N_j}{\partial x_j} \psi_j dR + \int_R K_{ij} k_{rw} \frac{\partial N_i}{\partial x_i} e_j dR \\
 & + \int_R \eta N_i N_j \frac{d\psi_j}{dt} dR - \int_B K_{ij} k_{rw} \left(\frac{\partial \psi}{\partial x_j} + e_j \right) n_i dB \\
 & - \int_R N_i q dR = 0, \quad I = 1, 2, \dots, n
 \end{aligned} \tag{3.2}$$

where R is the solution domain with boundary B , and n is the number of nodes in the finite element network.

Equation (3.2) can be written more concisely as

$$A_U \psi_I + B_U \frac{d\psi_I}{dt} = F_I, \quad I = 1, 2, \dots, n \tag{3.3}$$

where

$$A_U = \sum_e \int_{R^e} K_{ij} k_{rw} \frac{\partial N_i}{\partial x_i} \frac{\partial N_j}{\partial x_j} dR \tag{3.4a}$$

$$B_U = \sum_e \int_{R^e} \eta N_i N_j dR \tag{3.4b}$$

$$\begin{aligned}
F_I = & \sum_e \left(\int_{R^e} -K_{ij} k_{rw} \frac{\partial N_I}{\partial x_i} e_j dR \right) \\
& + \int_R N_I q dR + \sum_e \left(\int_{B^e} V_n N_I dB \right)
\end{aligned}
\tag{3.4c}$$

in which R^e is the element subdomain with boundary B^e , and V_n denotes the normal velocity at the boundary. The sign convention for V_n is the same as for q . That is, V_n is positive for inward flow and negative for outward flow.

In SAMFT2D, linear rectangular elements are used. For such elements, the element matrices can be evaluated efficiently using influence coefficient formulas given in Huyakorn et al. (1984).

3.2.2 Picard and Newton-Raphson Schemes

Equation (3.3) represents a system of n nonlinear ordinary differential equations. Time integration of these equations is performed using a fully implicit finite difference approximation. Two alternative nonlinear treatment procedures are provided in SAMFT2D. The first scheme is a Picard scheme that leads to a system of algebraic equations with symmetric coefficient matrix. The second scheme is a Newton-Raphson scheme that leads to a system of algebraic equations with asymmetric coefficient matrix. Both schemes are presented briefly in this section.

In the Picard scheme, equation (3.3) is approximated by the following equation:

$$\omega A_U^{k+\omega} \psi_J^{k+1} + (1-\omega) A_U^{k+\omega} \psi_J^k + \frac{B_U^{k+\omega}}{\Delta t_k} (\psi_J^{k+1} - \psi_J^k) = F_I^{k+\omega}, \quad I = 1, 2, \dots, n \quad (3.5)$$

where ω is a time-weighting factor, superscripts k and $k + 1$ are used to denote the previous and current time level respectively, and $\Delta t_k = t_{k+1} - t_k$. To obtain a fully implicit time-stepping scheme, the value of ω is set equal to 1. Equation (3.5) thus becomes:

$$(A_U^{k+1} + \frac{B_U^{k+1}}{\Delta t_k}) \psi_J^{k+1} = F_I^{k+1} + \frac{B_U^{k+1}}{\Delta t_k} \psi_J^k \quad (3.6)$$

which represents a symmetric matrix equation in view of the fact that both [A] and [B] are symmetric matrices. Nonlinear iterations are performed within each time step to achieve a stable numerical solution. The use of fully implicit (backward) difference time stepping combined with lumping (diagonalization) of storage matrix [B] proves to be advantageous for highly nonlinear situations where damping of oscillatory convergence behavior of the numerical solution is desirable.

In the Newton-Raphson scheme, equation (3.3) is replaced by the following integrated fully-implicit finite difference approximation:

$$G_I \equiv A_U \psi_J^{k+1} + B_U' (\psi_J^{k+1} - \psi_J^k) / \Delta t_k + E_U (S_{wJ}^{k+1} - S_{wJ}^k) / \Delta t = 0, \quad I=1, 2, \dots, n \quad (3.7)$$

where G_I is the nonlinear (vector array) function of the nodal head values, and B_{IJ}' and E_{IJ} are defined as

$$B_{IJ}' = \int_R S_s S_w N_I N_J dR \quad (3.8a)$$

$$E_{II} = \int_R \phi N_I dR \quad (3.8b)$$

$$E_{IJ} = 0 \text{ for } J \neq I \quad (3.8c)$$

Application of the Newton-Raphson procedure to (3.7) yields (see Huyakorn and Pinder, 1983):

$$G_I^{r+1} = G_I^r + \left(\frac{\partial G_I}{\partial \psi_J}\right)^r \Delta \psi_J^{r+1} = 0, \quad I=1,2,\dots,n \quad (3.9)$$

where r and $r+1$ denote previous and present iteration levels at the current time value,

$\Delta \psi_J^{r+1}$ is an iteration displacement vector defined as

$$\Delta \psi_J^{r+1} = \psi_J^{r+1} - \psi_J^r \quad (3.10)$$

and $(\partial G_I / \partial \psi_J)^r$ is the Jacobian of the Newton-Raphson iteration.

Equation (3.8) can be written in the form

$$H_{IJ}^r \psi_J^{r+1} = H_{IJ}^r \psi_J^r - G_I^r, \quad I=1,2,\dots,n \quad (3.11)$$

where $H_{IJ} = (\partial G_I / \partial \psi_J)^r$.

Owing to the fact that $[H]$ is an asymmetric matrix, (3.11) thus represents an asymmetric matrix equation. As in the Picard scheme, it is necessary to perform nonlinear iterations within the time step to achieve a stable numerical solution. Iterations are performed until the successive

change in pressure head values is within a prescribed tolerance. For each iteration, the Newton-Raphson scheme requires more than twice the computational effort compared with the Picard scheme. However, experience has indicated that the Newton-Raphson scheme with lumping of the storage matrix is more robust than the Picard scheme when dealing with highly nonlinear soil moisture characteristics.

Several convergence enhancement features have been implemented into the code and used in conjunction with both the Picard and the Newton-Raphson techniques. The first of such features is the use of extrapolation formulas for estimating nodal values, ψ_j^{k+1} thereby enhancing convergence of the iterative process. At the start of a new time level, an initial estimate of ψ_j^{k+1} is obtained from:

$$\begin{aligned}\psi_j^{k+1} &= \psi_j^k & , \text{ if } k = 1 \\ \psi_j^{k+1} &= \psi_j^k + (\psi_j^k - \psi_j^{k-1}) \Delta t_k / 2 \Delta t_{k-1} & , \text{ if } k = 2 \\ \psi_j^{k+1} &= \psi_j^k + (\psi_j^k - \psi_j^{k-1}) \frac{\log(t_{k+1}/t_k)}{\log(t_k/t_{k-1})} & , \text{ if } k > 2\end{aligned}\tag{3.12}$$

During subsequent iterations, improved estimates of ψ_j^{k+1} are obtained from

$$\psi_j^{k+1} = (1-\gamma) \psi_j^k + \gamma \psi_j^{r+1}\tag{3.13}$$

where γ is an underrelaxation factor ($0 < \gamma < 1$), and ψ_j^k and ψ_j^{r+1} are the current and previous iterations of nodal values of pressure head at the current time level, $k + 1$, respectively.

Another salient feature is the use of an automatic underrelaxation procedure to cope with oscillatory convergence behavior of the numerical solution. Via this procedure, the value of the

underrelaxation factor, γ , is computed as the iterations progress. The algorithm used to compute γ is adapted from Cooley (1983), and is given as

Step 1

$$S = \begin{cases} \frac{e_{r+1}}{e_r \gamma_{old}} & \text{if } r > 1 \\ 1 & \text{if } r = 1 \end{cases} \quad (3.14)$$

Step 2

$$\gamma_{new} = \begin{cases} \frac{3+s}{3+|s|} & \text{if } s \geq -1 \\ \frac{1}{2|s|} & \text{if } s < -1 \end{cases} \quad (3.15)$$

where r and $r + 1$ denote previous and current iteration levels, respectively, γ_{old} and γ_{new} are old and new values of the underrelaxation factor, and e is the absolute value of the largest difference between head values at two successive iteration levels ($e_r = \text{Max } |\psi_i^r - \psi_i^{r-1}|$).

The third convergence enhancement feature is the use of upstream weighting of relative permeability. This feature has been directly incorporated into the computation of element matrices for both the Picard and Newton-Raphson procedures. Via upstream weighting, the relative permeabilities for various elements are evaluated based on the flow direction.

The fourth feature is the use of chord slope formulas for evaluating gradients of water saturation versus head ($dS_w/d\psi$) and relative permeability versus water saturation (dk_{rw}/dS_w).

In addition to the mentioned convergence features, automatic time step reduction and marching procedure are utilized to handle convergence difficulties. Normally, for each specified (target) time step, the code will perform nonlinear iterations until the head values converge or

until the maximum allowable number of iterations (NITMAX) prescribed by the user is reached. If NITMAX is reached, and the solution has not converged, the computational time step is then reduced to 1/2 of the original target time step, and the iteration procedure is allowed to recommence. Should convergence be achieved, the simulation will continue using the reduced value of computational time step until the end of the target time step. If convergence still fails to occur, the computational time step is reduced further (by another 1/2 (i.e., now 1/4 of the target time step)). The iteration procedure is continued until either convergence is reached or the maximum allowable successive reductions of time step size (IRESOL) prescribed by the user is reached. The code will be halted if IRESOL value is reached with a warning message to the user.

3.2.3 Solute Transport

For the contaminant transport simulation, SAMFT2D solves (2.16) using an upstream-weighted residual finite element method. To illustrate the application of the technique, consider equation (2.15) and a trial solution for concentration be written in the form:

$$c(x_i, t) = N_j(x_i) c_j(t) \quad (3.16)$$

where $N_j(x_i)$ and $c_j(t)$ are the basis functions and nodal values of concentration at time t , respectively.

In the upstream weighted residual technique, the weighted residual integral equation is obtained using asymmetric (upstream) weighting functions (see Huyakorn and Nilkuha, 1979)

to weight the spatial derivative terms of the transport equation, and the standard basis functions to weight the remaining mass accumulation term. Application of this procedure to (2.15) yields

$$\int_R W_I \left[\frac{\partial}{\partial x_i} (D_{ij} \frac{\partial c}{\partial x_j} - V_i \frac{\partial c}{\partial x_i}) \right] - \int_R N_I \left[\phi S_w R \left(\frac{\partial c}{\partial t} + \lambda c \right) + q(c - c^*) \right] dR = 0 \quad (3.17)$$

where W_I are the upstream weighting functions.

Using Green's theorem to remove the second derivative and substituting for c , one obtains

$$\int_R (D_{ij} \frac{\partial W_I}{\partial x_i} \frac{\partial N_J}{\partial x_j} + V_i W_I \frac{\partial N_J}{\partial x_i}) c_J dR + \int_R \phi S_w R N_I N_J \left(\frac{dc_J}{dt} + \lambda c_J \right) dR + \int N_I q (c^* - N_J c_J) dR - \int_B W_I (D_{ij} \frac{\partial c}{\partial x_j} n_i) dB = 0 \quad (3.18)$$

Equation (3.18) can be expressed in the form

$$(E_U + B_U^*) c_J + \bar{B}_U \frac{dc_J}{dt} = \bar{F}_I \quad (3.19)$$

where

$$E_{ij} = \int_R (D_{ij} \frac{\partial W_I}{\partial x_i} \frac{\partial N_J}{\partial x_j} + V_i W_I \frac{\partial N_J}{\partial x_i}) dR \quad (3.20a)$$

$$\tilde{B}_U = \int_R (\phi S_w R) N_I N_J dR \quad (3.20b)$$

$$B_U^* = \int_R (\lambda \phi S_w R) N_I N_J dR \quad (3.20c)$$

$$\tilde{F}_I = - \int_R N_I q (c^* - N_J c_J) dR + \int_B W_I (D_{ij} \frac{\partial c}{\partial x_j}) n_i dB \quad (3.20d)$$

Once all of the element matrices have been computed and assembled into global matrices, the system of ordinary differential equations (3.19) can be integrated with respect to time. This leads to the following system of algebraic equations:

$$\left[\omega(E_U + B_U^*) + \frac{\tilde{B}_U}{\Delta t_k} \right] c_J^{k+1} = (\omega-1)(E_U + B_U^*) c_J^k + \frac{\tilde{B}_U}{\Delta t_k} c_J^k + \omega \tilde{F}_I^{k+1} + (1-\omega) \tilde{F}_I^k \quad (3.21)$$

where ω is the time weighting factor.

Equation (3.21) can be rearranged in the form:

$$G_U c_J^{k+1} = R_I^{k+1} \quad (3.22)$$

where

$$R_I^{k+1} = (\omega-1) (E_U + B_U^*) c_J^k + \frac{\bar{B}_U}{\Delta t_k} c$$

$$+ \omega \bar{F}_I^{k+1} + (1-\omega) \bar{F}_I^k$$
(3.23)

and

$$G_U = \omega(E_U + B_U^*) + \bar{B}_U/\Delta t_k$$
(3.24)

To obtain a second-order accuracy in time approximation, ω is chosen to be 0.5 thus yielding the Crank-Nicholson time stepping scheme. Equation (3.22) represents a system of linear algebraic equations with an asymmetric banded coefficient matrix.

3.2.4 Treatment of Boundary Conditions

The first-type boundary condition (2.20a) is treated by setting current concentration values at the boundary nodes to the prescribed concentration \bar{c} . Physically, the first-type boundary condition may apply to inflow boundary segments where the concentration of the incoming fluid is assumed to be approximately the same as the resident nodal concentration in the porous medium. Nodal points representing injection wells or contaminant sources may also be subject to the first type boundary condition if the stated equilibrium assumption is adopted.

The second-type boundary condition (2.20b) is treated by adding the integrated value of the prescribed dispersive flux to the right hand side of the discretized finite element equations. Physically, the second-type boundary condition may apply to impermeable boundary segments where the fluxes and normal concentration gradients are zero. It may also apply to certain

contaminant sources placed in an undisturbed flow field wherein the mass of waste material is leaching at a prescribed rate, q_c^D .

The third-type boundary condition (2.20c) generally applies to inlet boundary segments and/or injection wells when the concentration of incoming or injected fluid c^* may be unequal to the resident nodal concentration values. In this case, the integrated nodal values of the flux q_c^T are added to the right side of the finite element equations, and the integrated advective flux term corresponding to $v_i n_i c$ of (2.20c) is incorporated into the coefficient matrix. For the special case of pumping wells and outflow boundary, the outflow concentration c^* usually takes the same value as the resident nodal concentration, c . The boundary condition (2.20c) then reduces to that of (2.20b) with zero dispersive flux. This corresponds to the natural boundary condition of the finite element formulation used in the code and no treatment is needed.

A temporal variation of the boundary condition at any given node may be accommodated in a convenient manner by using either a continuous piecewise linear approximation or discontinuous (stepped) approximation of the actual graph of concentration or solute flux versus time.

3.2.5 Mass Balance Computation Schemes

As an option in the computer program, a mass balance calculation is provided at the end of each time step. For the flow equation, the mass balance over the whole solution region R is obtained by integrating equation (2.3) and applying Green's theorem to the spatial derivative terms. Thus, one obtains

$$\int_B K_{ij} k_{rw} \left(\frac{\partial \psi}{\partial x_j} + e_j \right) dB - \int_R \eta \frac{\partial \psi}{\partial t} dR + \int_R q dR = 0 \quad (3.25)$$

where

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

It should be noted that the first integral in equation (3.25) represents the net fluid flow across the whole boundary, the second integral represents the rate of volumetric storage in region R, and the last integral represents the net rate of volume production due to point sources and sinks.

If the exact solution of the flow equation is substituted into equation (3.25), the right hand side will be zero. However, if an approximate finite element solution ψ is substituted, the hand side of (3.25) will be non-zero, and will correspond to an error in material balance, ϵ_v

$$\epsilon_v = - \int_B V_i n_i dB - \int_R \eta \frac{\partial \psi}{\partial t} dR + \int_R q dR \quad (3.26)$$

where

$$q = \sum_{I=1}^{n_s} Q_I \delta(x - x_I) \quad (3.27a)$$

$$V_i = -K_{ij} k_{rw} \left(\frac{\partial \psi}{\partial x_j} + e_j \right) \quad (3.27b)$$

Next, we make use of the following properties of the basis functions:

$$\sum_{I^*=1}^{n_b} N_{I^*}(\tilde{x}^*) = 1 \text{ for all } \tilde{x}^* \text{ on } B \quad (3.28a)$$

and

$$\sum_{I=1}^n N_I(x) = 1 \text{ for all } x \text{ on } R \quad (3.28b)$$

where n_b is the number of nodes on the boundary and n is the total number of nodes in the whole solution region.

Combined equations (3.26)-(3.29) yields

$$\begin{aligned} \dot{e}_v = & \sum_{I^*=1}^{n_b} - \int_B N_{I^*} V_i n_i dB - \sum_{I=1}^n \int_R (\eta N_I N_J \frac{d\psi_J}{dt}) dR \\ & + \sum_{I^*=1}^{n_w} Q_{I^*} \end{aligned} \quad (3.29)$$

Equation (3.29) can be written in the form

$$\dot{e}_v = \sum_{I^*=1}^{n_b} -f_{I^*}^B - \sum_{I=1}^n f_I^S + \sum_{I^*=1}^{n_w} f_{I^*}^W \quad (3.30)$$

where

$$f_{I^*}^B = \int_B N_{I^*} V_i n_i dB \quad (3.31a)$$

$$f_I^S = \int_R \eta N_I N_J \frac{d\psi_J}{dt} dR \quad (3.31b)$$

$$f_{I^*}^W = Q_{I^*} \quad (3.31c)$$

The storage and sink and source terms in equation (3.30) are evaluated in a straightforward manner. The boundary integral terms, $f_{I^*}^B$, are evaluated by performing the

back-substitution of the Galerkin finite element equations at various boundary nodes. The procedure avoids the problem of discontinuities in the velocity field at the boundary nodes. Such discontinuities arise if one employs Darcy's Law to compute velocities at boundary nodes of individual elements and uses these velocities obtain f_{1*}^B .

After all the terms in (3.26) have been computed, the error in the rate of material balance, $\dot{\epsilon}_v$, can be determined. For each time level, the cumulative material balance error, $\epsilon_v^{t_{k+1}}$ is evaluated from

$$\epsilon_v^{t_{k+1}} = \sum_{l=1}^k \dot{\epsilon}_v \Delta t_l \quad (3.32)$$

A normalized form of ϵ_v is also determined using the following equation:

$$||\dot{\epsilon}_v|| = |\dot{\epsilon}_v| / \left[\sum_{I^*=1}^{n_b} |f_{I^*}| + \sum_{I=1}^n |f_s^I| + \sum_{I=1}^{n_w} |f_r^W| \right] \quad (3.33)$$

The solute mass balance calculation procedure is also performed in a similar manner to that already described for the fluid. First the integral form of the solute transport equation (2.15) is obtained

$$\int_B (D_{ij} \frac{\partial c}{\partial x_j} - V_i c) n_i dB - \int_R (\frac{\partial}{\partial t} (\phi S_w Rc) + \phi \lambda S_w Rc) dR + \sum_{I=1}^{n_w} Q_I c_I^* = 0 \quad (3.34)$$

This leads to the following expression for the rate of material balance error:

$$\begin{aligned}
\dot{\epsilon}_M = & \sum_{I^*=1}^{n_s} \int_B N_{I^*} (D_{ij} \frac{\partial c}{\partial x_j} - V_i c) n_i dB \\
& - \sum_{I=1}^n \int_R \phi S_w R N_I N_J (\frac{dc_I}{dt} + \lambda c_J) dR + \sum_{I^*=1}^{n_s} Q_I c_I^* \\
& - \sum_{I=1}^n \int_R N_I N_L c_L \eta N_J \frac{d\psi_J}{dt} dR
\end{aligned} \tag{3.35}$$

which can be expressed in the form

$$\dot{\epsilon}_M = - \sum_{I^*=1}^{n_s} F_{I^*}^B - \sum_{I=1}^n f_I^s + \sum_{I^*=1}^{n_s} F_I^w \tag{3.36}$$

where

$$F_{I^*}^B = \int_B N_{I^*} (V_i c - D_{ij} \frac{\partial c}{\partial x_j}) n_i dB \tag{3.37a}$$

$$f_I^s = \int_R \phi S_w R N_I N_J (\frac{dc_I}{dt} + \lambda c_J) dR + \sum_{I=1}^n \int_R N_L c_L (\eta n_I N_J \frac{d\psi_J}{dt}) dt \tag{3.37b}$$

$$F_I^w = Q_I c_I^* \tag{3.37c}$$

Except for the boundary integral term, all other terms in equation (3.35) can be evaluated in the straightforward manner. The evaluation of the boundary material flux is more involved and requires further elaboration. In a case involving a third type boundary condition, the total material flux distribution is prescribed as

$$(V_i c - D_{ij} \frac{\partial c}{\partial x_j}) n_i = q_c^T \quad (3.38)$$

and thus, $F_{I^*}^B$ is given explicitly by

$$F_{I^*}^B = \int_B N_{I^*} q^T dB \quad (3.39)$$

In a case involving a second type boundary condition, the outward dispersive flux distribution is prescribed as

$$-D_{ij} \frac{\partial c}{\partial x_j} n_i = q_c^D \quad (3.40)$$

and the outward advective flux is obtainable from

$$V_i n_i c = q N_j c_j \quad (3.41)$$

where q is the outward normal fluid flux distribution. Equations (3.40) and (3.41) are combined with equation (3.39) to yield

$$\begin{aligned} F_{I^*}^B &= \int_B N_{I^*} (q N_j c_j + q_c^D) dB \\ &\approx c_{I^*} \int_B N_{I^*} q dB + \int_B N_{I^*} q_c^D dB \end{aligned} \quad (3.42)$$

where the summation convention is not applied to subscript I^* , and the fluid integral corresponds to the nodal fluid flux at boundary node I^* .

In a case involving a first type boundary condition, the dispersive boundary nodal flux is not known explicitly and should be computed by back-substitution of c into the original finite

element approximation of the transport equation at node I^* . Once the dispersive nodal flux Q_{cl}^D has been computed the total boundary nodal flux may be obtained from

$$F_{I^*}^B \approx c_{I^*} \int_B N_{I^*} q dB + Q_{cl}^D \quad (3.43)$$

Finally, when all the various material flux terms have been computed, the error in the rate of material balance, $\dot{\epsilon}_M$, can be determined from equation (3.36). In practice, the cumulative mass balance error at a current time level, $\epsilon_M^{t_{k+1}}$ should also be computed. It is given by

$$\epsilon_M^{t_{k+1}} = \sum_{\ell=1}^k (\dot{\epsilon}_M \Delta t_\ell) \quad (3.44)$$

Both $\epsilon_M^{t_{k+1}}$ and its normalized form $E_M^{t_{k+1}}$ are used as indicators of the global accuracy of the numerical solution of the transport equation. For convenience, we define $E_M^{t_{k+1}}$ as

$$E_M^{t_{k+1}} = \sum_{\ell=1}^k (\dot{\epsilon}_M \Delta t_\ell) / \left(\sum_{\ell=1}^n F_I^S \right) \quad (3.45)$$

3.3 NUMERICAL TREATMENT OF MULTIPHASE PROBLEMS

3.3.1 Discretized Finite Element Equations

The Galerkin finite element procedure with a fully implicit time integration is applied to the multiphase flow equations represented by (2.21). This leads to a system of nonlinear algebraic equations of the form:

$$\left[A'_{IJ} \Phi_{IJ} \right]^{t+\Delta t} + \frac{B'_{II}}{\Delta t} \left[(\rho_t \theta S_t)_{II}^{t+\Delta t} - (\rho_t \theta S_t)_{II}^t \right] = \dot{M}_{II}^{t+\Delta t} \quad (3.46)$$

for $I = 1, 2, \dots, n$

where n is the number of nodes in the finite element grid, and A'_{IJ} and B'_{II} are fluid transmissivity and storage coefficient matrices. Note that the storage matrix B'_{II} is diagonalized by applying a standard lumping procedure.

Assuming that compressibilities of the porous matrix and the liquid phases are negligible, equation (3.46) may be rewritten for a three-phase flow situation as follows:

$$A'_{IJ} \Phi_{wJ} + \frac{B'_{II}}{\Delta t} \left[\rho_w \Delta^t S_{wI} \right] - \dot{M}'_{wI} = 0 \quad (3.47a)$$

$$A'_{IJ} \Phi_{nJ} + \frac{B'_{II}}{\Delta t} \left[\rho_n \Delta^t S_{nI} \right] - \dot{M}'_{nI} = 0 \quad (3.47b)$$

$$A'_{IJ} \Phi_{aJ} + \frac{B'_{II}}{\Delta t} \left[\Delta^t (\rho_a S_a)_{II} \right] - \dot{M}'_{aI} = 0 \quad (3.47c)$$

where

$$B'_{II} = \theta_I B'_{II} \quad (3.48a)$$

$$\Phi_{wJ} = p_{wJ} + \rho_w gZ \quad (3.48b)$$

$$\Phi_{nJ} = p_{nJ} + \rho_n gZ \quad (3.48c)$$

$$p_{nJ} = p_{wJ} + \bar{p}_{cnw} \quad (3.48d)$$

and

Δ^t is a time increment operator defined as

$$\Delta^t f = f^{t+\Delta t} - f^t \quad (3.48e)$$

Note that the nodal value of air potential may be evaluated as follows:

$$\Phi_{aJ} = \rho_{aJ} \int_{p_{am}}^{p_{aJ}} \frac{d\xi}{\rho_a} + \rho_{aJ} gZ \quad (3.49a)$$

Assuming that the equation of state for ideal gas may be used, the integral in (3.49a) is given by

$$\int_{p_{am}}^{p_{aJ}} \frac{d\xi}{\rho_a} = \int_{p_{am}}^{p_{aJ}} \frac{d\xi}{\beta_a p_a} = \frac{1}{\beta_a} \ln \left(\frac{p_{aJ}}{p_{am}} \right) \quad (3.49b)$$

where p_{aJ} is assumed to be greater than zero, and β_a is the compressibility of the gas phase. For an ideal gas $\beta_a = M/RT$.

To avoid numerical integration, we elect to use bilinear rectangular elements and express the element matrices as follows:

$$A_{IJ}^l \Phi_{IJ} = \sum_{J \in \eta_l} \tau_{IJ}^u \gamma_{IJ} (\Phi_{IJ} - \Phi_{IJ}) \quad , l = w, n, a \quad (3.50)$$

and

$$B_{II} = (Lm/4)\Theta_I \quad (3.51)$$

where η_I is a vector array containing the nodal numbers of the nodes reconnected to node I, τ_{IJ} is an upstream mobility value that depends on the flow direction between nodes I and J of the rectangular element considered, γ_{IJ} is a transmissivity coefficient connecting nodes I and J, L and m are the length and width of the element, respectively, and Θ_I is the value of effective porosity at node I.

The upstream mobility value τ_{IJ}^u is computed using the following algorithm:

$$\tau_{IJ}^u = \left[\frac{1 - \omega_{IJ}^l}{2} \right] \tau_{II} + \left[\frac{1 + \omega_{IJ}^l}{2} \right] \tau_{IJ} \quad (3.52)$$

$$J = \eta_{IJ} \quad (3.53a)$$

$$\omega_{IJ}^l = -|\omega| \text{ if } \gamma_{IJ} (\Phi_{II} - \Phi_{IJ}) \geq 0 \quad (3.53b)$$

$$\omega_{IJ}^l = |\omega| \text{ if } \gamma_{IJ} (\Phi_{II} - \Phi_{IJ}) < 0$$

where τ_{II} and τ_{IJ} are mobility values at nodes I and J, respectively, and $|\omega|$ is the absolute upstream factor normally set equal to 1 for full upstream weighting.

3.3.2 Treatment of Nonlinearities by Newton-Raphson Scheme

Consider a general situation where all three fluid phases (water, NAPL and air) are active. For this situation, the selected primary variables for three-phase flow are p_n , S_n and S_w , and the nodal residual equations are written in the form:

$$R_I^w(p_{nI}, S_{nI}, S_{wI}) = 0 \quad (3.54a)$$

$$R_I^n(p_{nI}, S_{nI}, S_{wI}) = 0 \quad (3.54b)$$

$$R_I^a(p_{nI}, S_{nI}, S_{wI}) = 0 \quad (3.54c)$$

where R_I^w , R_I^n and R_I^a correspond to the left hand side of equations (3.47a) - (3.47c), respectively.

Application of the Newton-Raphson procedure to (3.54a) - (3.54c) yields:

$$\frac{\partial R_I^w}{\partial p_{nJ}} \Delta p_{nJ} + \frac{\partial R_I^w}{\partial S_{nJ}} \Delta S_{nJ} + \frac{\partial R_I^w}{\partial S_{wJ}} \Delta S_{wJ} = -(R_I^w)^k \quad (3.55a)$$

$$\frac{\partial R_I^n}{\partial p_{nJ}} \Delta p_{nJ} + \frac{\partial R_I^n}{\partial S_{nJ}} \Delta S_{nJ} + \frac{\partial R_I^n}{\partial S_{wJ}} \Delta S_{wJ} = -(R_I^n)^k \quad (3.55b)$$

$$\frac{\partial R_I^a}{\partial p_{nJ}} \Delta p_{nJ} + \frac{\partial R_I^a}{\partial S_{nJ}} \Delta S_{nJ} + \frac{\partial R_I^a}{\partial S_{wJ}} \Delta S_{wJ} = -(R_I^a)^k \quad (3.55c)$$

where

$$\Delta p_{wJ} = p_{nJ}^{k+1} - p_{nJ}^k \quad (3.56a)$$

$$\Delta S_{nJ} = S_{nJ}^{k+1} - S_{nJ}^k \quad (3.56b)$$

$$\Delta S_{wJ} = S_{wJ}^{k+1} - S_{wJ}^k \quad (3.56c)$$

and k and $k+1$ denote previous and current iteration levels, respectively.

In SAMFT2D, a second formulation considering the three-phase fluid system but with two active phases (water and NAPL) is also provided. The selected primary variables of the water and NAPL flow equations are p_w and S_n , and the nodal residual equations are written in the form:

$$R_I^w(p_{wl}, S_{nl}) = 0 \quad (3.57a)$$

$$R_I^n(p_{wl}, S_{nl}) = 0 \quad (3.57b)$$

Application of the Newton-Raphson procedure to equations (3.57a) and (3.57b) yields:

$$\frac{\partial R_I^w}{\partial p_{wj}} \Delta p_{wj} + \frac{\partial R_I^w}{\partial S_{nj}} \Delta S_{nj} = -(R_I^w)^k \quad (3.58a)$$

$$\frac{\partial R_I^n}{\partial p_{wj}} \Delta p_{wj} + \frac{\partial R_I^n}{\partial S_{nj}} \Delta S_{nj} = -(R_I^n)^k \quad (3.58b)$$

A third Newton-Raphson formulation is also available for a simpler two-phase situation of NAPL flow in the saturated zone of the groundwater system. The selected primary variables for this case are p_w and S_w , and the nodal residual equations are written in the form:

$$R_I^w(p_{wl}, S_{wl}) = 0 \quad (3.59a)$$

$$R_I^n(p_{wl}, S_{wl}) = 0 \quad (3.59b)$$

Application of the Newton-Raphson procedure to equations (3.59a) and (3.59b) yields:

$$\frac{\partial R_I^w}{\partial p_{wj}} \Delta p_{wj} + \frac{\partial R_I^w}{\partial S_{wj}} \Delta S_{wj} = -(R_I^w)^k \quad (3.60a)$$

$$\frac{\partial R_I^n}{\partial p_{wj}} \Delta p_{wj} + \frac{\partial R_I^n}{\partial S_{wj}} \Delta S_{wj} = -(R_I^n)^k \quad (3.60b)$$

3.3.3 Treatment of Boundary Conditions

Prescribed flux boundary conditions are treated simply by adding the specified nodal flux values to the right-hand side of the corresponding nodal equations. To ensure non-zero diagonal

coefficients, the water-phase equations are replaced by the phase-summed equations. It should be noted that a zero diagonal can occur in the water-phase equation for node I if water-phase mobility values at node I and its neighbors are zero.

Prescribed pressure boundary conditions are treated using the procedure described by Forsyth (1988). The method incorporates a prescribed condition $p_{II} = \bar{p}$ by first simulating a no-flow situation of the node and then using a source/sink term, Λ_I^l to inject or produce the correct amount of fluid so that p_{II} approaches \bar{p} . The residual equation for flow of phase l at node I is thus written in the form:

$$R_I^l + \Lambda_I^l = 0 \quad (3.61)$$

where R_I^l is as obtained previously from the discretization of the governing operation without a source/sink term. Physically, we regard Λ_I^l as the mass flux of phase l through a thin skin layer of porous material adjacent to the boundary portion covered by node I. If we impose the prescribed pressure on the exterior surface of the skin layer and assume negligible gravitational effect, and zero storage in the skin layer, then Λ_I^l may be evaluated as follows:

$$\Lambda_I^l = A_I k_s \tau_l (p_{II} - \bar{p}) / b_s \quad (3.62)$$

where A_I is the effective flow area of node I, k_s and b_s are the permeability and thickness of the skin, and τ_l is an upstream phase mobility evaluated as follows:

$$\tau_l = \tau_{II} \quad \text{if } (p_{II} > \bar{p}) \quad (3.63a)$$

and

$$\tau_t = \tau_t (S_t = 1) \quad \text{if } (\bar{p} \geq p_{tI}) \quad (3.63b)$$

The modified residual equation is now rewritten in the form:

$$R_t' + Wk_s \tau_t (p_{tI} - \bar{p}) \quad (3.64)$$

where

$$k_s = \max (k_{xI}, k_{yI}, k_{zI}) \quad (3.65a)$$

and

$$W = (A_i/b_s) \quad (3.65b)$$

In order to ensure that the converged numerical solution meets the criterion: $p_{tI} - \bar{p} \leq \epsilon_p$ (Pressure tolerance), we need to make W a large number but not so large as to induce unacceptable round-off errors in mass balance computation. The following empirical formula for determining W has been found to work well:

$$W = 1000 * \max_{\forall I} (\Delta x_i) / \min_{\forall I} (\Delta y_i) \quad (3.66)$$

3.3.4 Nonlinear Iteration and Time Stepping Schemes

In solving a multiphase flow problem, iterations must be performed within each time step to obtain a stable numerical solution. During each iteration, nodal values of the primary variables are updated for the next iteration. If necessary, time step adjustments are made to handle a convergence problem and obtain an efficient transient simulation.

The updating of the nodal values of the unknown variables is performed using a scheme with an under-relaxation factor determined automatically and dependent upon the maximum

convergence errors for the entire mesh. The following relaxation formula is used to obtain improved estimates of the nodal unknowns:

$$x_i^{r+1} = x_i^r + \Omega^{r+1} \Delta x_i^{r+1} \quad (3.67)$$

where x_i the nodal unknown variables (p_{nl} , S_{nl} , S_{wl} in a case of three-phase flow), $r+1$ and r denote current and previous iterations, respectively, and Ω^{r+1} is a relaxation factor for the current iterate.

The value of Ω^{r+1} is determined from:

$$\Omega^{r+1} = \min [\Omega_p^{r+1}, \Omega_s^{r+1}] \quad (3.68)$$

subject to

$$0.1 \leq \Omega^{r+1} \leq 1 \quad (3.69)$$

where Ω_p^{r+1} and Ω_s^{r+1} are the relaxation factors associated with convergence errors in the pressure and saturation variables, respectively. Ω_p^{r+1} is determined using the algorithm of Cooley (1983), described in Section 3.2.

Ω_s^{r+1} is determined using the following formula:

$$\Omega_s^{r+1} = \min \left[\frac{0.2}{|e_s^{r+1}|}, 1 \right] \quad (3.70)$$

where

$$|e_s^{r+1}| = \max \left[\max_I |\Delta S_{\ell}^s|, \ell = w, n, a \right] \quad (3.71)$$

with S_ℓ denoting saturation of phase ℓ .

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

- (1) Start the numerical solution for the first time step with a specified value of Δt_1 . Perform the nonlinear Newton-Raphson (or Picard) iterations. If satisfactory convergence is obtained, then determine the subsequent computational time steps using the following algorithm used by Forsyth (1990):

$$\Delta t_{k+1} = TMUL * \Delta t_k \leq \Delta t_{\max}, k \geq 1 \quad (3.72)$$

where Δt_{\max} is the maximum allowable time step size prescribed a priori, and TMUL is the time step multiplier. The value of TMUL is given by:

$$TMUL = \min \left[\frac{DPWISH}{|\Delta^i p|_{\max}}, \frac{DSWISH}{\sum |\Delta^i S_\ell|_{\max}} \right]; \ell = \text{active phases} \quad (3.73a)$$

subject to:

$$0.0001 \leq TMUL \leq 5 \quad (3.73b)$$

where

$$|\Delta' p|_{\max} = \max_I |p_I^{k+1} - p_I^k| \quad (3.74a)$$

$$|\Delta' S_t|_{\max} = \max_I |S_{II}^{k+1} - S_{II}^k| \quad (3.74b)$$

and desired incremental changes in pressure and saturation values over the time step.

- (2) If convergence difficulty is encountered (i.e., solution fails to converge within the allowable maximum number of nonlinear iterations, NITMAX), then reduce the computational time step size according to the following scheme:

$$\Delta t_k = \Delta t_k / TDIV \quad (3.75)$$

where TDIV is the time step divider.

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

3.3.5 Mass Balance Computational Schemes

As an option in the multiphase flow module of the code, a mass balance calculation is performed at the end of each specified time step. Mass balance error information is provided for water and NAPL, which are the dominant fluid phases. The computational procedure is similar to that described in Section 3.2.5 for a single-phase flow simulation.

3.4 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. Presently, an algorithm is incorporated into SAMFT2D which allows the code to account for hysteresis effects for a single-phase flow simulation. This algorithm needs to be extended for application to multiphase flow problems. The algorithm is presented in this Section. It 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.

A typical hysteretic $S(p)$ relation is shown in Figure 3.1 and will be referred to illustrate the calculation procedure. The figure shows the main drainage, $S^d(p)$, and the main imbibition, $S^w(p)$, 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_{\max}^0 and S_{\min}^0 (Note: saturations may be scaled such that $S_{\max}^0 = 1$ and $S_{\min}^0 = 0$, however this does not need to be the case). The boundary $S(p)$ curves are described by

$$S^d(p) = S_{\min}^0 + (S_{\max}^0 - S_{\min}^0) F^d(p) \quad (3.76a)$$

$$S^i(p) = S_{\min}^0 + (S_{\max}^0 - S_{\min}^0) F^i(p) \quad (3.76b)$$

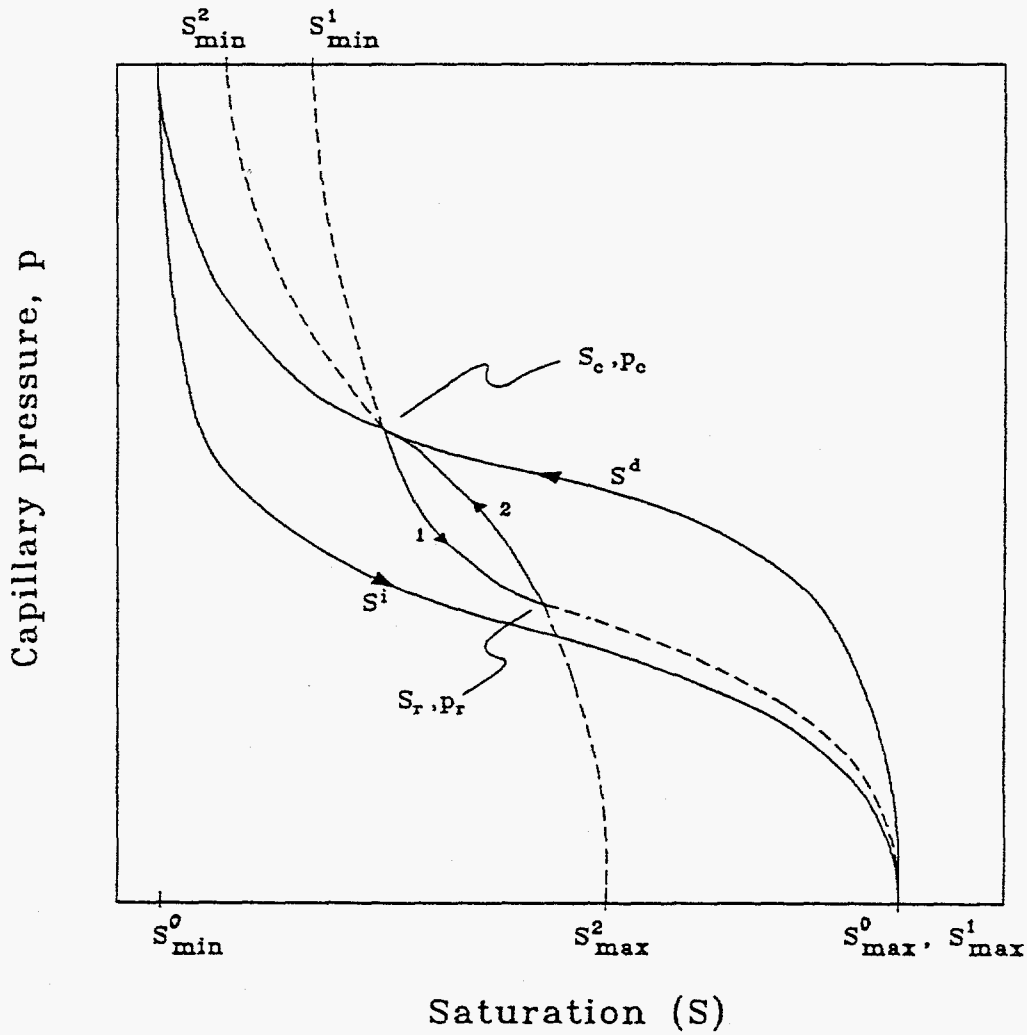


Figure 3.1. Typical hysteretic saturation - capillary pressure relation.

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).

$$F^d(p) = [1 + (\alpha^d p)^{\beta^d}]^{-\gamma^d} \quad (3.77a)$$

and

$$F^i(p) = [1 + (\alpha^i p)^{\beta^i}]^{-\gamma^i} \quad (3.77b)$$

with

$$\gamma = 1 - 1/\beta \quad (3.77c)$$

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

$$S^1(p) = S_{\min}^1 + (S_{\max}^1 - S_{\min}^1) F^i(p) \quad (3.78a)$$

and

$$S^2(p) = S_{\min}^2 + (S_{\max}^2 - S_{\min}^2) F^d(p) \quad (3.78b)$$

The parameters S_{\min}^1 , S_{\max}^1 , S_{\min}^2 , and S_{\max}^2 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_{\max}^1 is given by $S_{\max}^1 = S_{\max}$. Conversely, for all primary drainage curves the value of S_{\min}^1 is given by $S_{\min}^1 = S_{\min}$.

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:

$$S(p) = S_{\min}^2 + (S_{\max}^2 - S_{\min}^2) F^d(p) \quad (3.79)$$

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

$$S(p_r) = S_r = S_{\min}^2 + (S_{\max}^2 - S_{\min}^2) F^d(p_r) \quad (3.80a)$$

and

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

Equation (3.80) can be rewritten as

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

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

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

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

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

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 $F^i(\theta)$ is used instead of $F^d(\theta)$. 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 $[S_r, p_r] = [S_{\min}^0, p_{\min}]$ and $[S_c, p_c] = [S_{\max}^0, p_{\max}]$. The corresponding parameters for the main drainage curve are $[S_r, p_r] = [S_{\max}^0, p_{\max}]$ and $[S_c, p_c] = [S_{\min}^0, p_{\min}]$. 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 3.1, 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 3.1, this means that upon continued drainage, the main drainage boundary $S^d(p)$ is followed.

Implementation of the above algorithm 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 (3.76a) is written as

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

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

$$\mathcal{F}(S) = \frac{1}{\alpha} [S^{-1/\gamma} - 1]^{1/\beta} \quad (3.85)$$

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

3.5 NUMERICAL TREATMENT OF MULTIPHASE TRANSPORT PROBLEMS

The formulation for multiphase transport of a single contaminant component has been presented in Section 2.3.2, and the governing equation is given as equation (2.59). The equation contains extra terms describing the fate of precipitated mass in addition to the standard terms for advection, dispersion, sorption and decay. In a similar manner to that presented for single-phase transport, the multiphase transport equation is discretized using the upstream-weighted residual finite element procedure. This leads to a system of linear algebraic equations of the form:

$$\begin{aligned} \left[\Theta(E_{IJ} + B_{IJ}^*) + \frac{\tilde{B}_{IJ}}{\Delta t_k} \right] c_j^{k+1} &= \left[(\Theta - 1)(E_{IJ} + B_{IJ}^*) + \frac{\tilde{B}_{IJ}}{\Delta t_k} \right] c_j^k \\ &+ \Theta \tilde{F}_I^{k+1} + (1 - \Theta) \tilde{F}_I^k + \frac{B'_{IJ}}{\Delta t_k} [(m)_J^{k+1} - (m)_J^k] \\ &+ B'_{IJ} \lambda [\Theta m_j^{k+1} + (1 - \Theta) m_j^k] \end{aligned} \quad (3.86)$$

where Θ is the time weighting factor, and for the sake of convenience, subscripts w and p and the contaminant injection terms have been dropped. The coefficient matrices E_{IJ} , \tilde{B}_{IJ} and B_{IJ}^* and the right-hand side vector \tilde{F}_I can be readily obtained from those given in equations (3.20a) - (3.20d) for single-phase transport. The coefficient matrix B'_I is simply defined as:

$$B'_{IJ} = \int_R N_I N_J dR \quad (3.87)$$

Equation (3.86) may be rearranged to give:

$$G_{IJ} c_j^{k+1} + H_{IJ} m_j^{k+1} = R_I \quad (3.88)$$

Note that equation (3.88) appears to have two nodal unknowns (c_j^{k+1} and m_j^{k+1}). However, these unknowns are mutually exclusive and there always is only one unknown at each node at one time. The system of algebraic equations can be reorganized so that only the primary unknowns at the $k+1$ time level appear on the left-hand side. The modified system of equations may be represented by:

$$G_{IJ}^* u_j^{k+1} = -H_{IJ}^* v_j^{k+1} + R_I \quad (3.89)$$

where u_j^{k+1} and v_j^{k+1} are combinations of c_j^{k+1} and m_j^{k+1} , and contain only unknown and known variables at the current time level.

The matrices $[G^*]$ and $[H^*]$ are derived from $[G]$ and $[H]$ by combining appropriate columns. Once the solution to the equation (3.89) is obtained, the constraint relations (2.60) and (2.61) 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 $[G^*]$ and $[H^*]$ are modified by exchanging the appropriate columns. The new 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.

4 EXAMPLE VERIFICATION AND APPLICATION PROBLEMS

4.1 GENERAL

Four sets of test problems were used for verification of numerical schemes and demonstration of major capabilities of the single-phase and multiphase modules of the SAMFT2D code. The first two sets of problems concern water flow and solute transport in variably saturated porous media. These problems are as follows:

- Transient drainage and infiltration in a soil column with hysteresis
- Two-dimensional flow in a vertical section of a soil slab
- Transient two-dimensional flow in a root zone
- Steady-state two-dimensional flow beneath a landfill
- One-dimensional horizontal transport in a soil slab
- Two-dimensional transport in a soil slab
- Two-dimensional transport in uniform groundwater flow
- Leachate migration from a sanitary landfill.

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
- Vertical two-phase flow in a three-phase fluid system
- Vertical three-phase flow
- Two-dimensional migration of NAPL in a variably saturated groundwater system

- Two-dimensional migration of NAPL in a fully saturated groundwater system
- Multiphase 1-D transport of a contaminant component in a soil column
- Multiphase 2-D transport of a contaminant component in an unconfined aquifer system.

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.

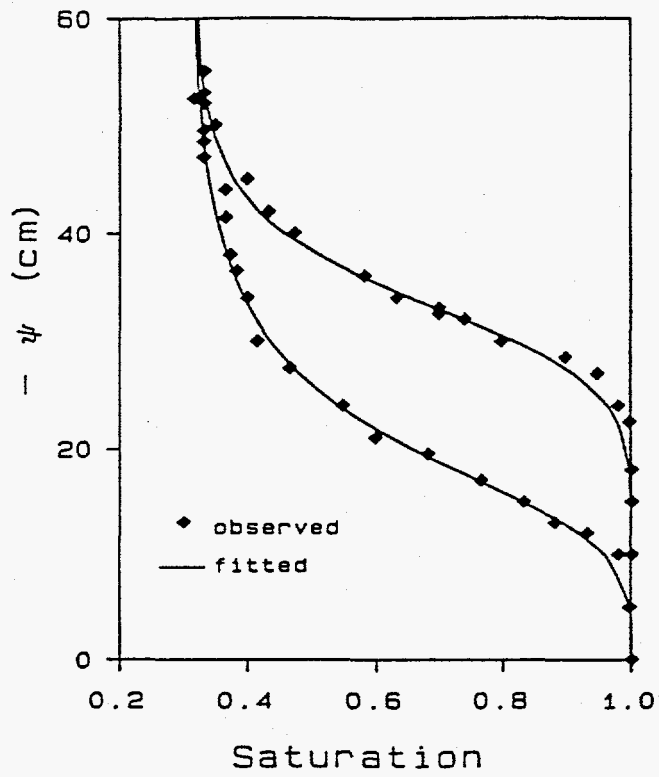
4.2 SINGLE-PHASE FLOW PROBLEMS

4.2.1 Transient Drainage and Infiltration in a Soil Column with Hysteresis

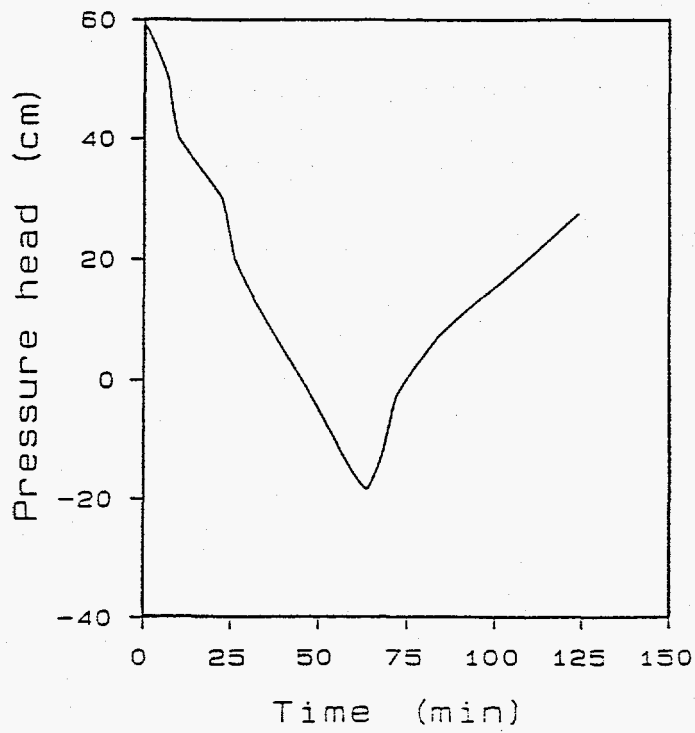
This problem involves transient, one-dimensional single-phase flow in a vertical column. The problem simulated is the slow drainage rewet experiment described by Gillham et al. (1979). In this example the soil moisture relationship (Figure 4.1a) exhibits considerable hysteresis. The depicted data points 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 4.1. 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 4.1b. The imposed variations in bottom boundary pressure



(a)



(b)

Figure 4.1. Hysteretic saturation-pressure head data and bottom boundary conditions used in the simulation.

Table 4.1 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

head cause the column to drain (along the boundary drying curve), followed by rewetting (along primary wetting curves) after $t = 60$ minutes. The SAMFT2D simulation of this experiment is shown in Figure 4.2. The data points in this figure represent measured saturations at $t = 68$ min and $t = 125$ min. Saturation profiles predicted by SAMFT2D are represented by the solid lines. The dashed curve represents simulation results obtained using the VAM2D computer code (Huyakorn et al., 1989). The measured data in Figure 4.2 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 SAMFT2D 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.

4.2.2 Two-Dimensional Flow in a Cross Section of 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 two-dimensional case involving gravity effect. The problem, solved previously using three other codes (VAM2D and UNSAT2), is described schematically in Figure 4.3. As illustrated, a rectangular soil slab, with sectional dimensions of 15 cm by 10 cm and a width of 10 cm, had an initial pressure head of -90 cm. The boundary conditions depicted in Figure 4.3 were then applied and maintained thereafter. The soil properties used in the simulation are the same as those presented in Section

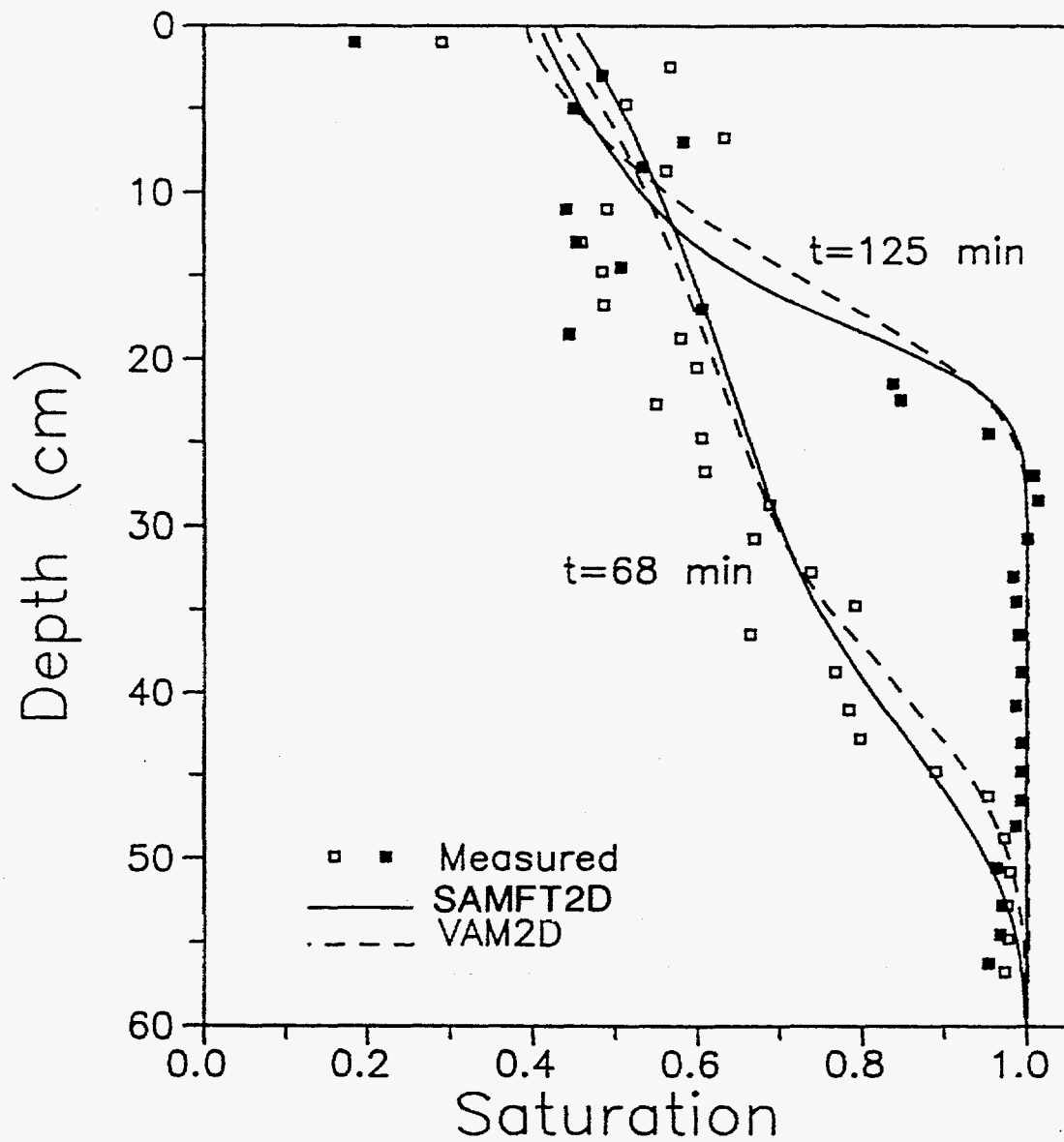


Figure 4.2. Observed and simulated water saturation in soil column for problem 4.2.4. Data points represent measured data; solid and dashed lines represent SAMFT2D and VAM2D results, respectively.

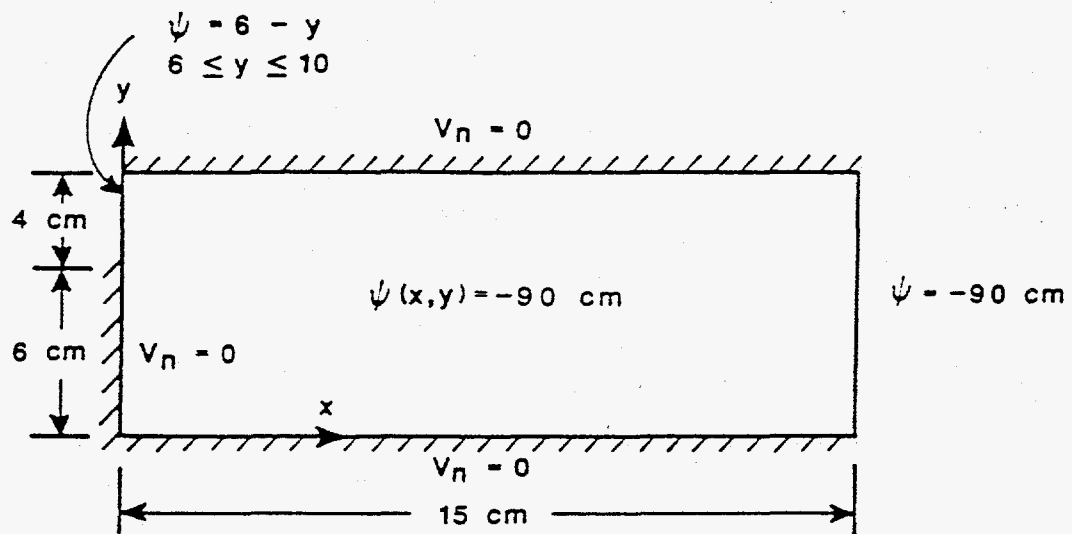


Figure 4.3. Geometry and boundary conditions used in the simulation of 2-D unsaturated flow in a soil slab.

4.2.1 for the horizontal flow problem.

The flow region was discretized using a rectangular grid consisting of 150 elements and 176 nodes. A constant nodal spacing was used along each coordinate axis. The nodal spacings in the x and y directions were $\Delta x = 1$ cm and $\Delta y = 1$ cm, respectively. The simulation was performed for 15 time steps. Time-step values were generated within the code using the algorithm: $\Delta t_1 = 864$ s, $\Delta t_k = 1.2\Delta t_{k-1} \leq 4320$ s for $k = 2, \dots, 15$. The numerical solution was obtained using the nonlinear Picard iteration scheme without mass lumping of the storage matrix. The maximum allowable error for pressure head was specified as 0.01 cm.

The number of nonlinear iterations required for convergence (within the prescribed tolerance of 0.01 cm) varies from 3 to 6 over the 15 time steps of simulation. Computed values of pressure head on the base and the top of the flow region are plotted in Figure 4.4 for a time value of 43200 s (0.508 days). Also included in the numerical solution obtained from UNSAT2, the two-dimensional Galerkin finite element code, documented in Neuman et al. (1974) and Davis and Neuman (1983). It can be seen that there is good agreement between the two numerical solutions.

4.2.3 Transient Vertical Flow 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 4.5. The purpose is to demonstrate another application of SAMFT2D to a different type of field problem. The modeled root zone is 100 cm thick and comprised of three layers with contrasting hydraulic properties. Although this particular problem is only one-dimensional, it was analyzed using a rectangular grid consisting

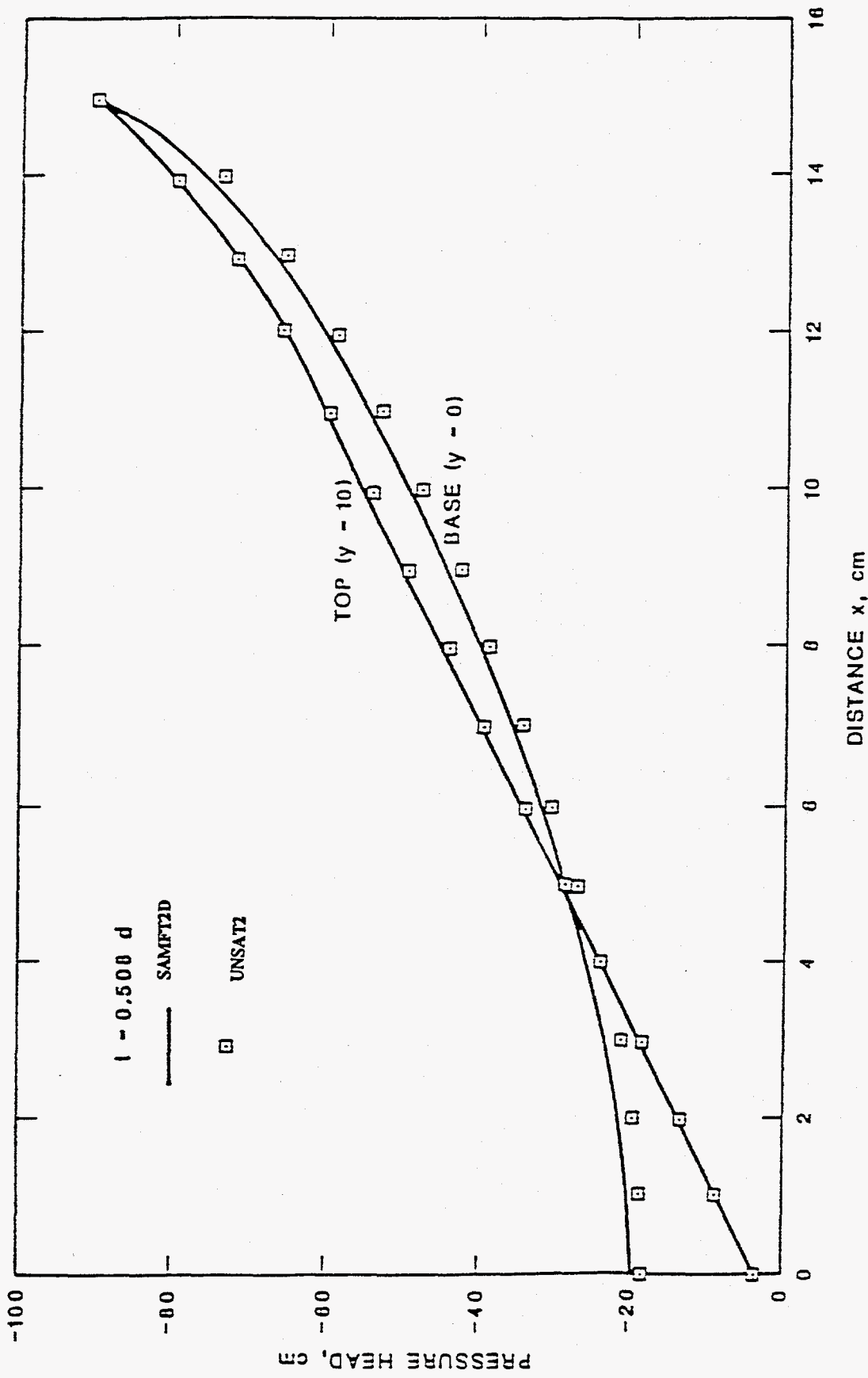


Figure 4.4. Pressure head distributions along the base and the top of the flow region.

$$v_n = I(t)$$

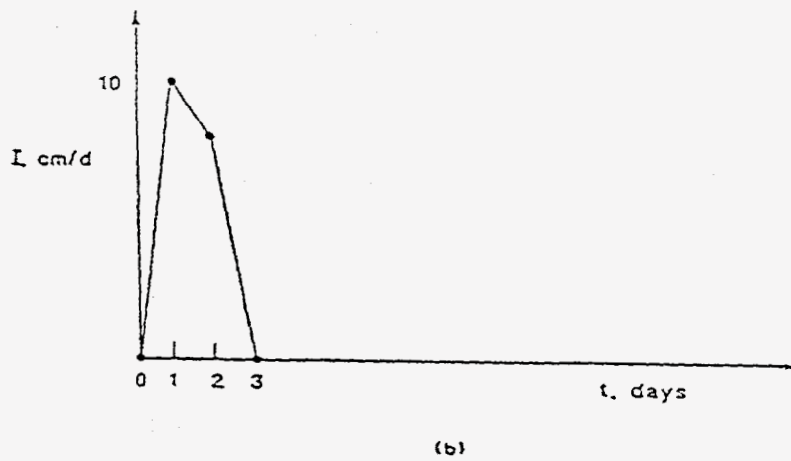
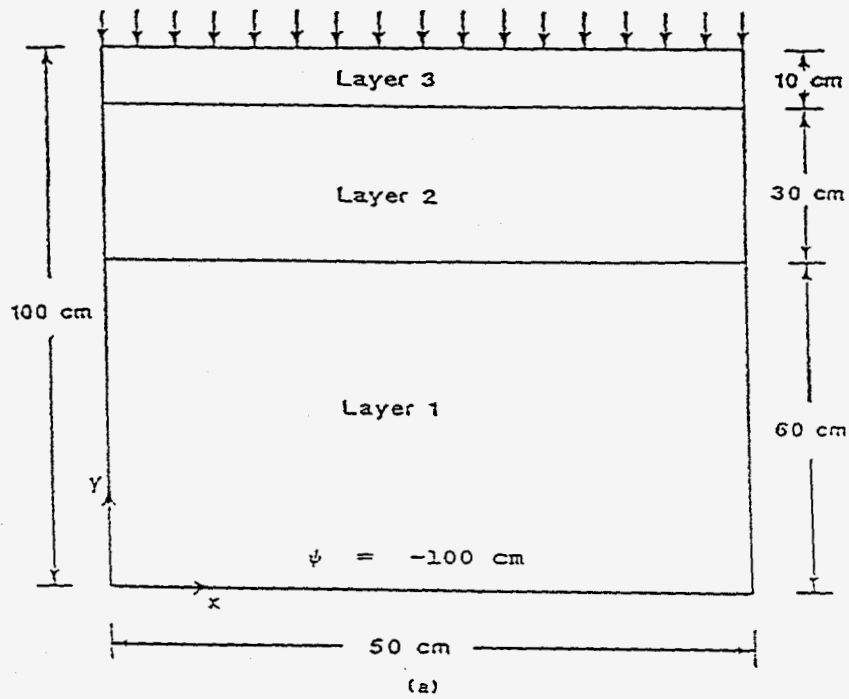


Figure 4.5. Schematic description of the root zone problem.

of 256 nodes (16 rows and 16 columns of nodes). 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 4.6 and 4.7 are pressure head and water saturation profiles, respectively. The ability of the SAMFT2D code to accommodate rapid response and contrasting properties of the soil system may be noted.

4.2.4 Steady-State Two-Dimensional Flow Beneath a Landfill

This problem, solved previously using the VAM2D and VADOFT 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 4.8 is required before a transient simulation of leachate migration from the landfill can be made. The hydraulic properties of the aquifer are assumed to be homogeneous and isotropic. The hydraulic conductivity, K , and the effective porosity, ϕ , are 750 m/yr and 0.25, respectively. The constitutive relations used to describe soil moisture characteristics in the vadose zone are as follows:

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

and

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

Note that the soil moisture relations for this particular problem are highly nonlinear. A rectangular grid consisting of 651 nodes and 600 elements was set up to represent the flow

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:

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

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

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

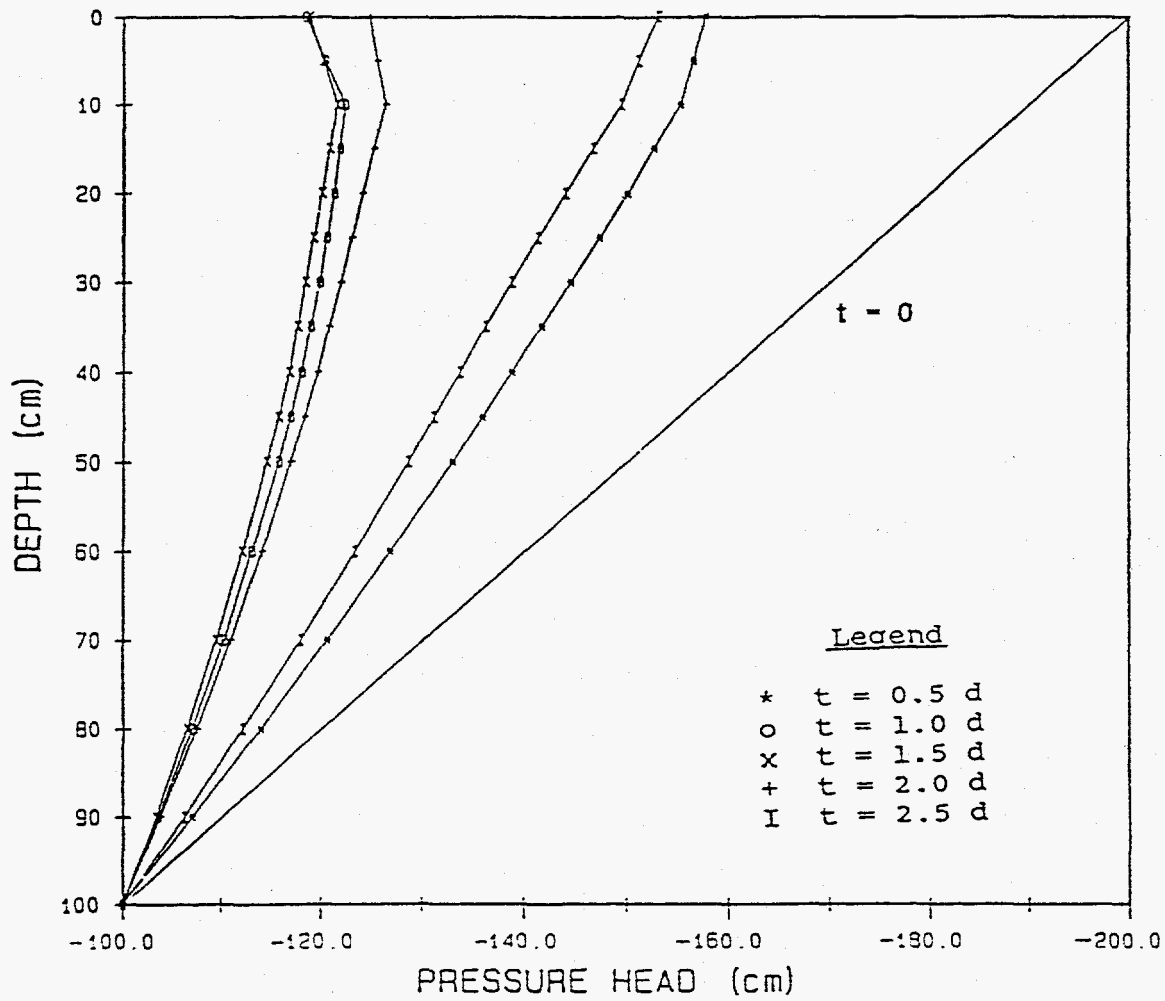


Figure 4.6. Simulated profiles of pressure head in the root zone.

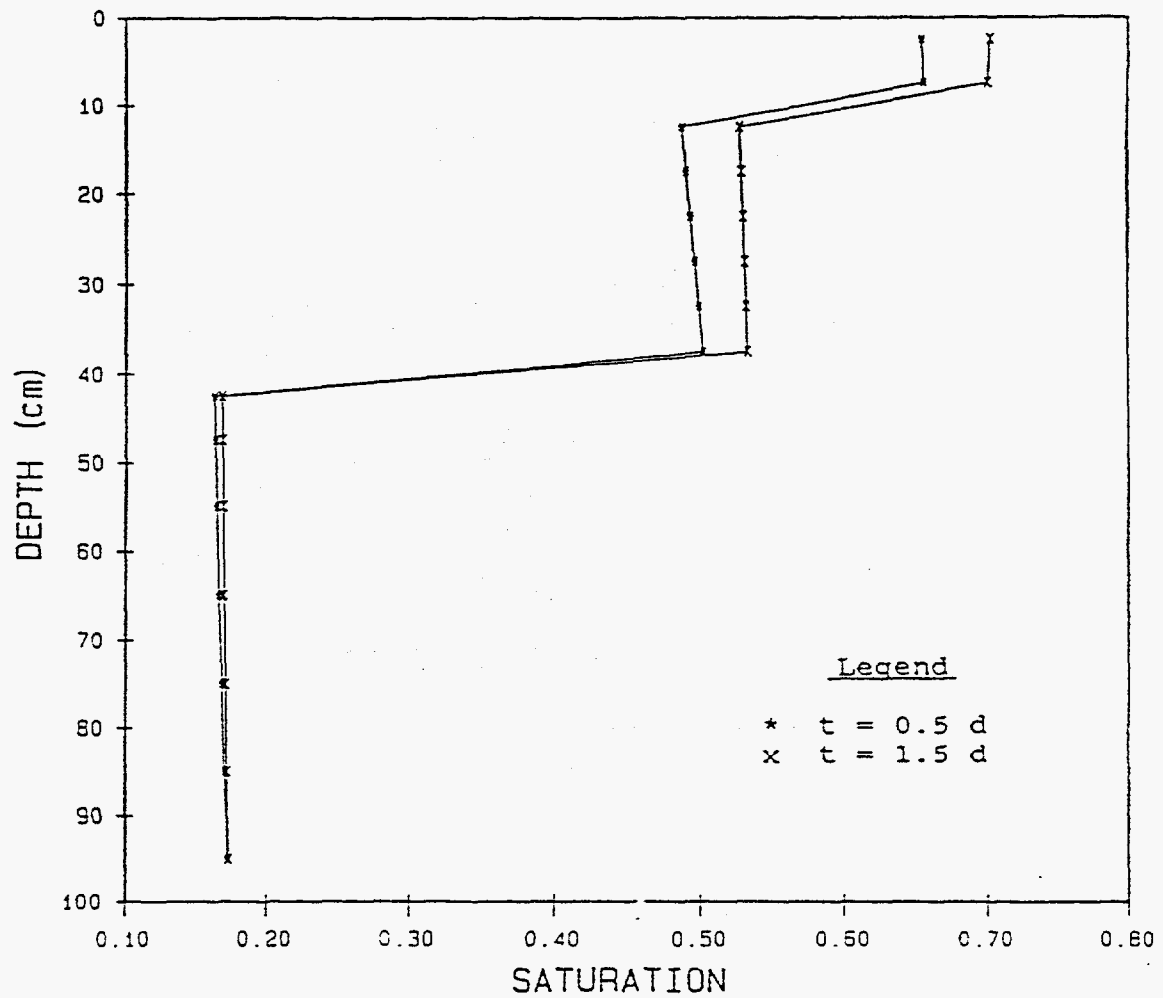


Figure 4.7. Simulated profiles of water-phase saturation in the root zone.

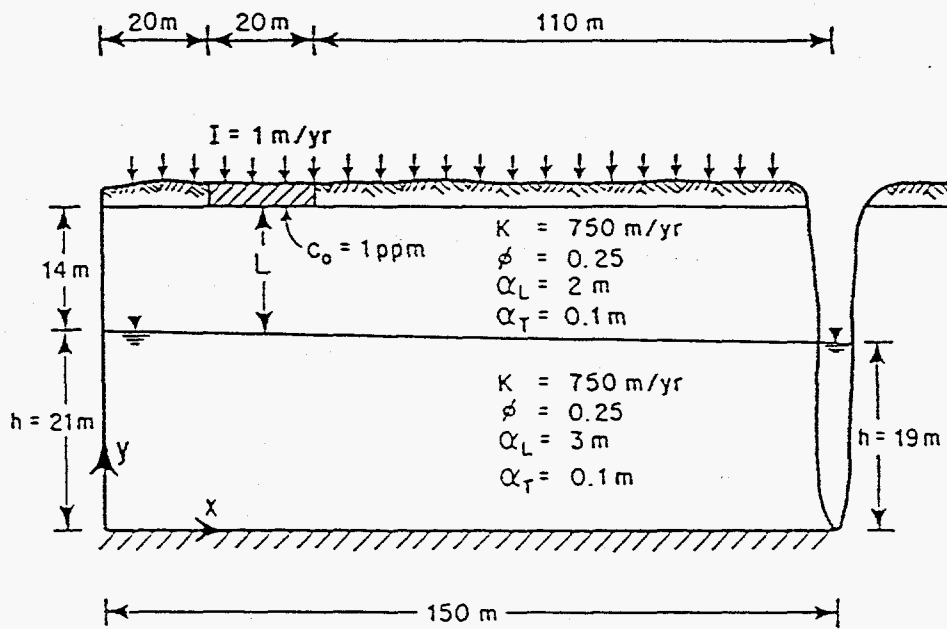


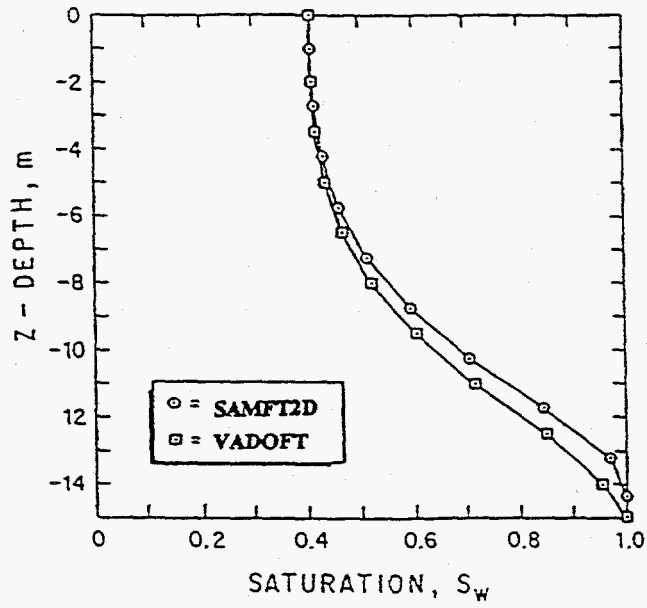
Figure 4.8. Schematic description of the simulated case of water flow and leachate migration in an unconfined system beneath a landfill.

region. The nodal spacings in the x and y directions were kept uniform and equal to 5 m and 1.75 m, respectively. 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 4.9 are simulation results. For the vertical section directly below the center of land disposal unit, water saturation profiles computed by SAMFT2D and a simplified one-dimensional finite element code (VADOFT, documented by Huyakorn et al., 1987) are compared in Figure 4.9a. There is reasonable agreement between the two-dimensional (SAMFT2D) and the one-dimensional (VADOFT) numerical solutions. It can be seen in Figure 4.9b, flow in the unsaturated zone is vertically dominant up to a depth of approximately 5 m above the water table. As the water particle approaches the water table its flow direction becomes laterally dominated. This deviation from the strict one-dimensional flow assumption used in the VADOFT code is likely to be the cause of the difference in the two saturation profiles depicted in Figure 4.9a.

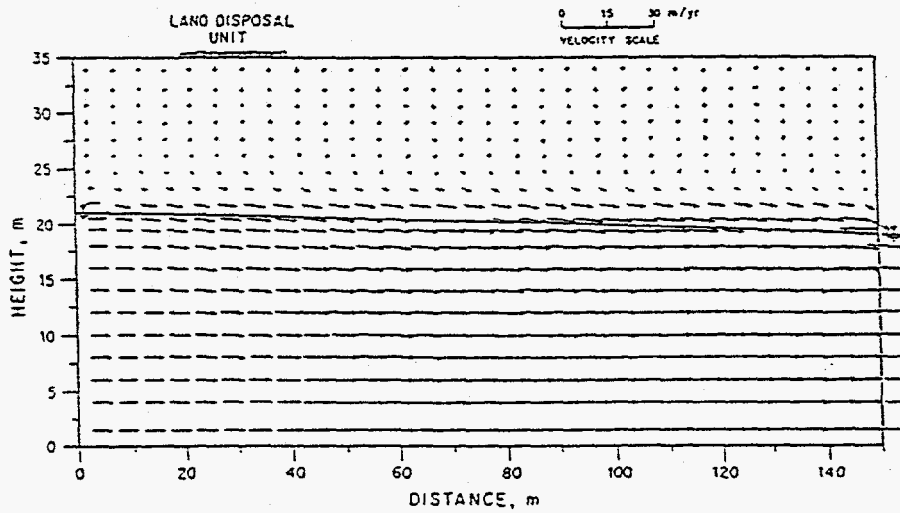
4.3 SINGLE-PHASE TRANSPORT PROBLEMS

4.3.1 One-Dimensional Transport in a Soil Slab

The purpose of this problem is to test the coding of the finite element formulation for a one-dimensional case involving advective-dispersive transport in an unsaturated porous medium. The problem concerns transient one-dimensional moisture movement and transport of a non-conservative species in an unsaturated soil slab. Velocities were obtained by solving the horizontal unsaturated flow problem and used as input data for the current transport problem.



(a)



(b)

Figure 4.9. Simulated saturation profiles and velocity field.

Initial and boundary conditions required for the flow and transport simulations are depicted in Figure 4.10. The physical parameter values are presented in Table 4.3.

The numerical solution was obtained using a mesh consisting of 20 rectangular elements, each with $\Delta x = 1$ cm. The problem was run for 20 time steps with a constant value of $\Delta t = 864$ s (0.01 days). Typical velocity profiles used in the transport calculation are illustrated in Figure 4.11. It is important to recognize that for the unsaturated flow case considered, the velocity distribution is time-dependent and this fact must be taken into account in the mass balance calculation to avoid obtaining an incorrect result. Computed concentration profiles at 0.04 and 0.2 days are depicted in Figure 4.12.

4.3.2 Two-Dimensional Transport in a Soil Slab

This problem concerns transport of a nonconservative solute in a rectangular cross section of an unsaturated soil. It corresponds to the 2-D unsaturated flow problem described in Section 4.2.2. As illustrated in Figure 4.13, the soil is initially dry and water and solute are allowed to enter the system at the upper portion of the left-hand boundary, $x = 0$ and $6 \leq y \leq 10$ cm. The right-hand boundary, which corresponds to the outlet, is maintained at the same initial pressure head value. At the inlet, the pressure head is maintained at $\psi = 6 - y$, and the solute concentration is assumed to be 1 ppm. No flow and zero normal concentration gradients are applied to the remaining portions of the entire boundary.

Values of the physical parameters required are given in Table 4.4. Values of water saturation and Darcy velocities at different times were determined by analyzing the associated flow problem. Both flow and transport were simulated using a medium rectangular grid. The

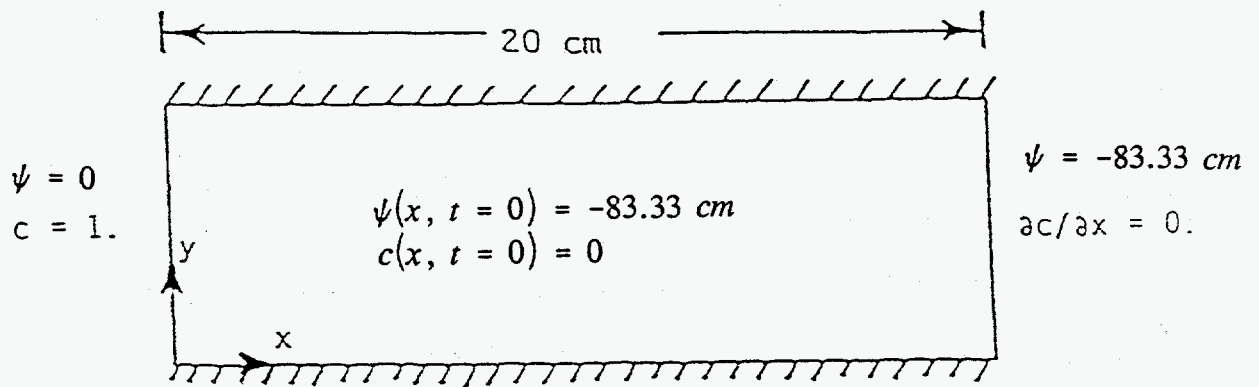


Figure 4.10. Schematic description and data for the problem of transport in an unsaturated soil slab.

Table 4.3. Values of physical parameter used in the simulation of 1-D transport in a soil slab ($p_w = \rho_w g \psi$).

Intrinsic permeability, k	1.157E-10	cm ²
Porosity, ϕ	0.45	
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^0	-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
Initial concentration, c_0	0	
Longitudinal dispersivity, α_L	1	cm
Apparent molecular diffusion, D_0	1.15E-7	cm ² /s
Retardation coefficient, R	2	
Degradation coefficient, λ	1.15E-8	s ⁻¹

Moisture retention functions:

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

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

where $S_{wr} = 0.333$.

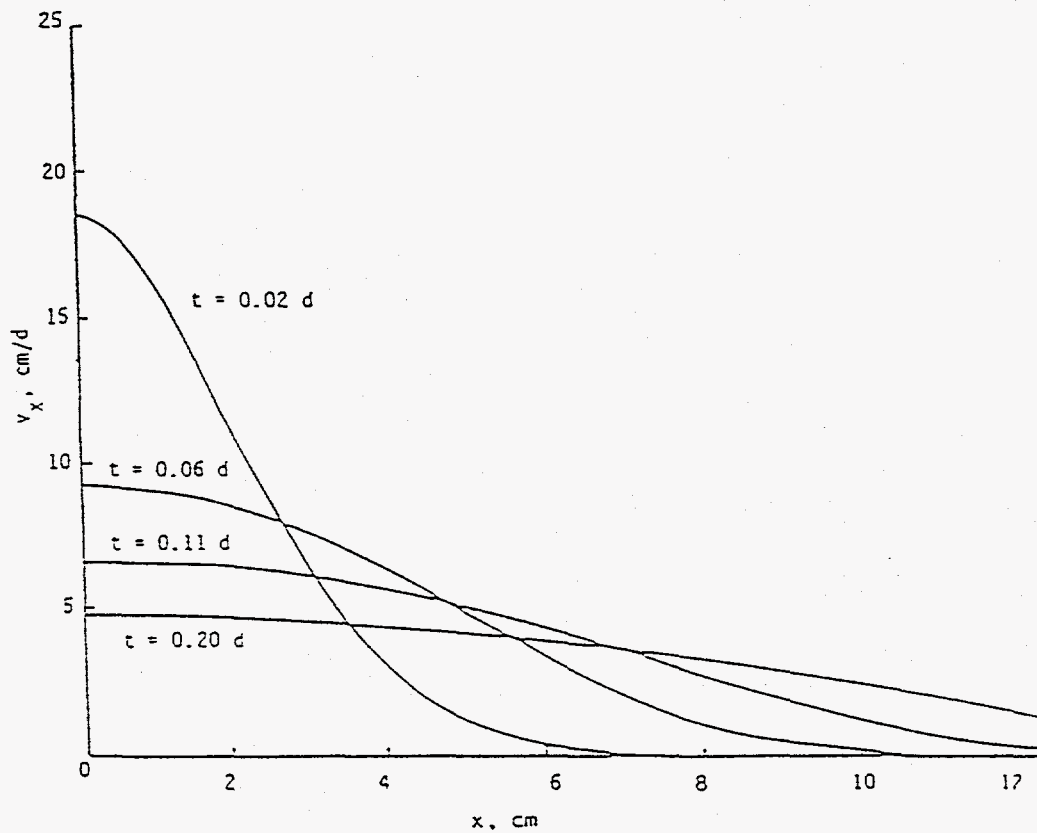


Figure 4.11. Typical velocity profiles used in the one-dimensional transport analysis.

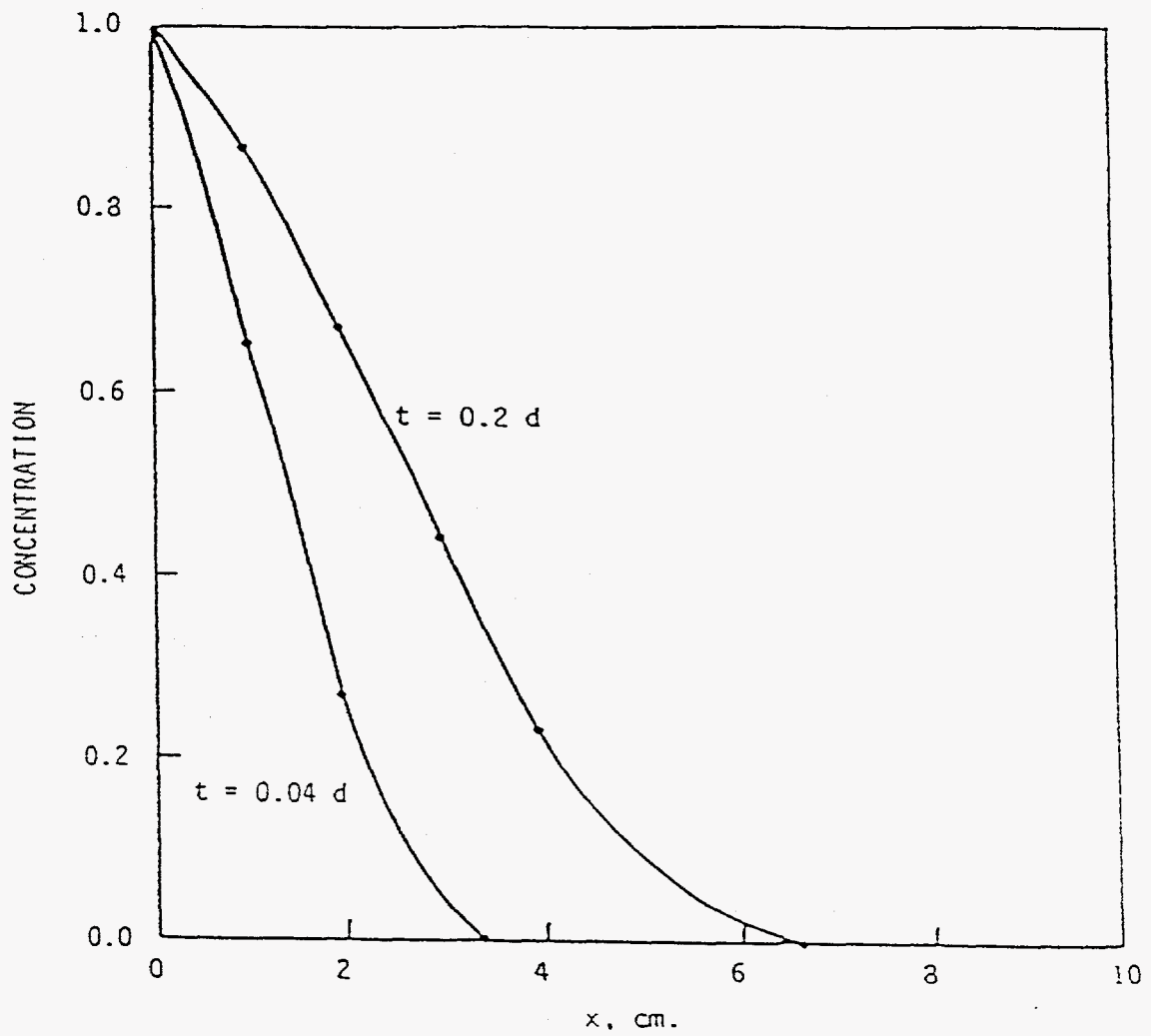


Figure 4.12. Simulated concentration profiles for the one-dimensional transport problem.

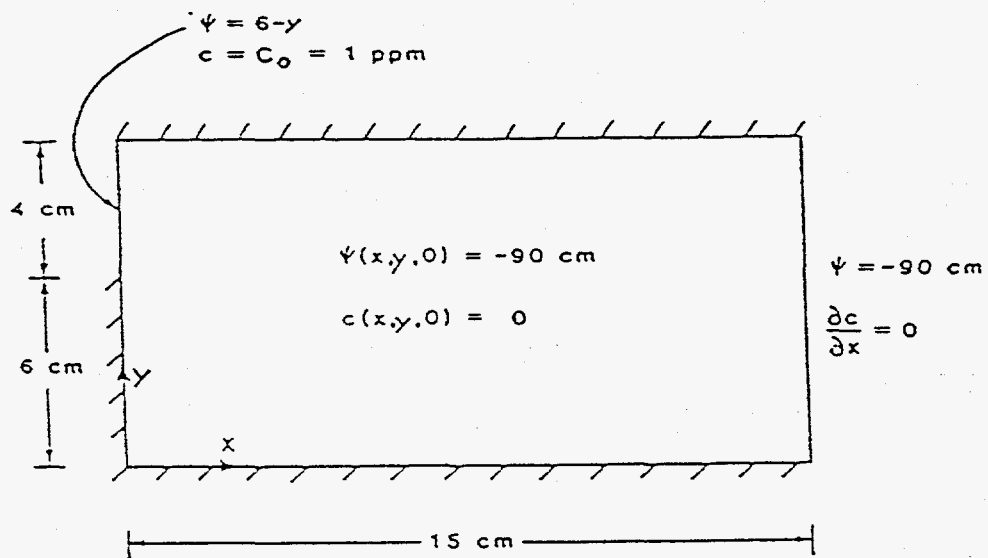


Figure 4.13. Schematic description and data for the problem of two-dimensional transport in a soil slab.

Table 4.4. Values of physical parameters used in the simulation of 2-D transport in a soil slab.

Parameter	Value
Hydraulic conductivity, K	1 cm/d
Porosity, ϕ	0.45
Initial pressure head, ψ_0	-90 cm
Initial concentration, c_0	0
Longitudinal dispersivity, α_L	1 cm
Transverse dispersivity, α_T	0 cm
Apparent molecular diffusion, D_0	0.01 cm ² /d
Decay coefficient, λ	0.001 d ⁻¹
Bulk density, ρ_B	1.46 g/cm ³
Distribution coefficient, k_d	0.308 cm ³ /g

Soil moisture relations used are the same as those given in Section 4.3.1.

grid was a uniform 11 x 16 grid comprised of 176 nodes and 150 elements. The nodal spacings were $\Delta x = \Delta y = 1$ cm. Time increment values were generated within the code using the algorithm: $\Delta t_1 = 864$ s (0.01 days), $\Delta t_k = 1.2\Delta t_{k-1} \leq 4320$ s (0.05 days).

The transport simulation was performed for 15 time steps using the Galerkin scheme. (Upstream weighting was not applied in this case because the cell Peclet number, $Pe = \Delta x/\alpha_L$, was not large enough to create numerical oscillations.) For verification purposes, the solution obtained using the present finite element model is compared in Figures 4.14 and 4.15 with the corresponding Galerkin solution obtained using the FEMWASTE code (Yeh and Ward, 1981). Evidently, the overall agreement between the two numerical solutions is reasonable. The horizontal concentration distributions depicted in Figure 4.14 are all smooth, although the profile predicted by the present model appears to be slightly ahead of that predicted by FEMWASTE. Note, however, that at the two later time values the vertical concentration distributions computed by FEMWASTE exhibit undesirable oscillations and incorrect representation of the zero normal gradient boundary condition at the top boundary, $y = 10$ cm. In contrast, the vertical concentration profiles computed by the present model are smooth. Furthermore, the zero normal gradient condition at $y = 10$ cm is very well duplicated.

4.3.3 Two-Dimensional Transport in Uniform Groundwater Flow

This problem was solved previously by using several other finite element codes (e.g., SEFTRAN, VAM2D and SAFT3D). It concerns two-dimensional dispersion of solute species released from a point source in the horizontal plane of uniform groundwater flow. The problem was selected to test the transport numerical schemes in the SAMFT2D in two dimensions.

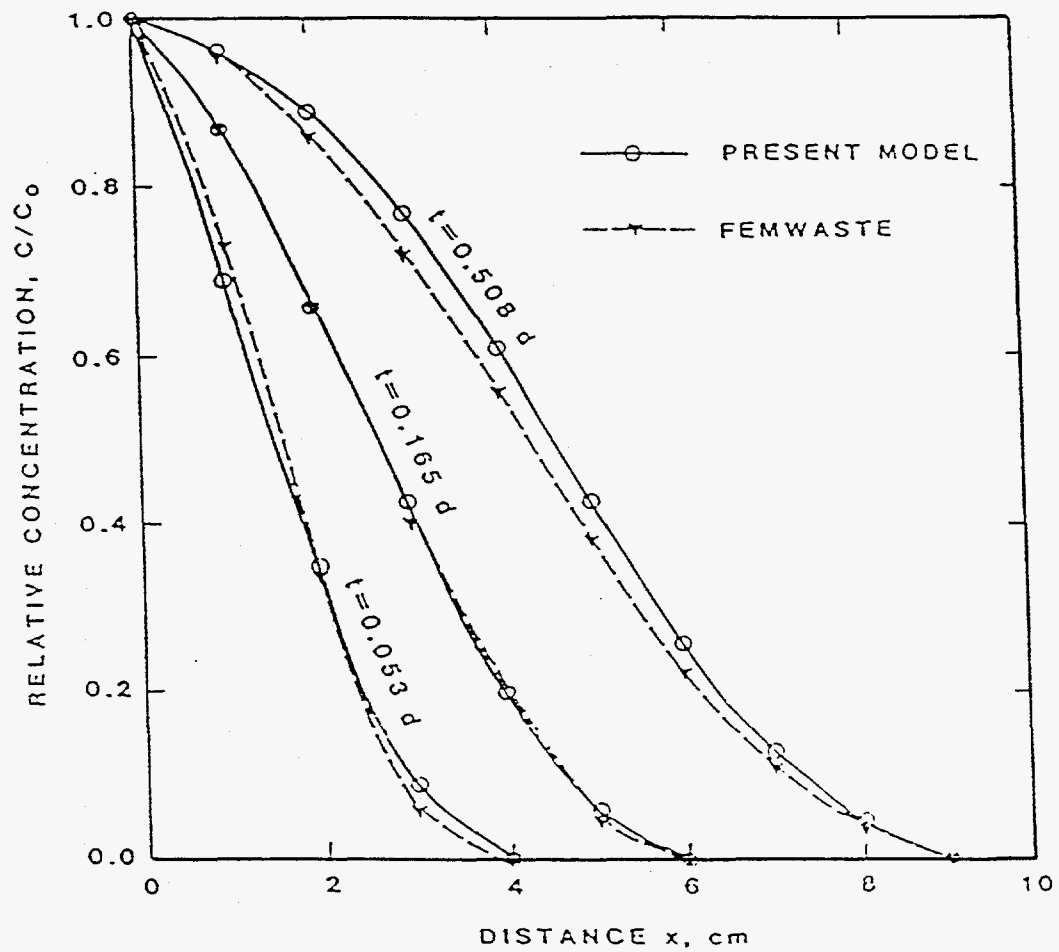


Figure 4.14. Computed horizontal profiles for typical time values.

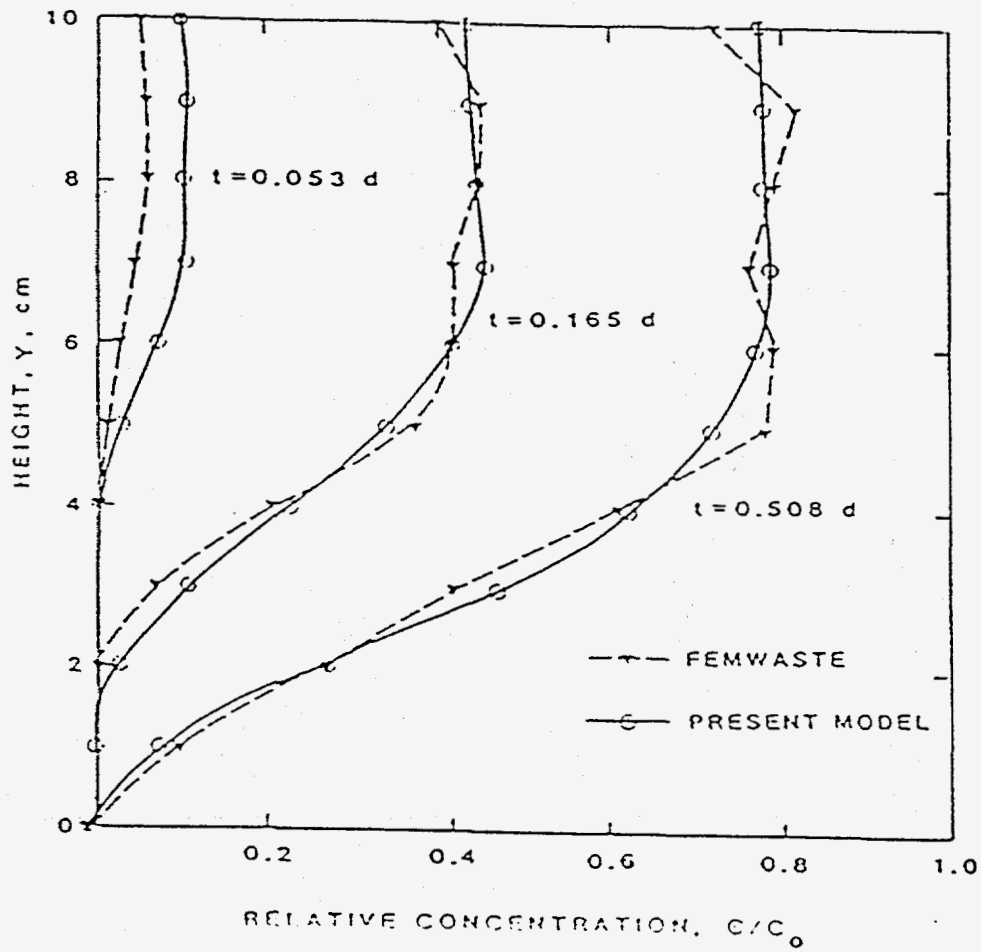


Figure 4.15. Computed vertical profiles for typical time values.

Parameter values used to run the code are listed in Table 4.5. A medium uniform grid consisting of 440 nodes and 390 rectangular elements was used. The grid with $\Delta x = 60$ m and $\Delta y = 30$ m is bounded by $-360 \leq x \leq 1980$ m and $0 \leq y \leq 300$ m. It represented the upper half of the modeled flow region because of symmetry about the x-axis. Two cases corresponding to degrading and nondegrading species were simulated. In each case, the standard Galerkin scheme with central difference time stepping was used, and the simulation was performed for 28 time steps with $\Delta t = 100$ d. It was assumed that the contaminant source was non-decaying and contaminant leaching occurred at a uniform rate of $Qc_0 = 704$ g/d per unit aquifer thickness. Results obtained are depicted in Figures 4.16 and 4.17. The numerical solutions from SAMFT2D are compared with the single-component analytical solution presented by Wilson and Miller (1978). Note that the concentration profiles along the x-axis (plume center line) are plotted in dimensionless form with the given definition of dimensionless variables. As can be seen, the numerical and analytical solutions are in fairly good agreement. In Figure 4.17, the numerical result obtained using a fine mesh with $\Delta x = 60$ m and $\Delta y = 15$ m is also presented to illustrate the convergence behavior of the numerical solution. The case simulated corresponds to a field situation involving transport of hexavalent chromium. Observed plume data reported by Perlmutter and Lieber (1970) is compared with the SAMFT2D simulation result as shown in Figure 4.18. Considering the uncertainties in the values of the transport parameters used in the simulation, the agreement between the predicted and observed plumes is quite reasonable.

Table 4.5. Parameter values used in the simulation of 2-D transport in uniform groundwater flow.

Parameter	Value
Darcy velocity, V	0.161 m/d
Porosity, ϕ	0.35
Longitudinal dispersivity, α_L	21.3 m
Transverse dispersivity, α_T	4.3 m
Aquifer saturated thickness, b	33.5 m
Contaminant mass flux, Qc_0 (per unit thickness of aquifer)	704 g/(m.d)
Bulk density, ρ_B	1.46 g/cm ³
Decay coefficient, λ case 1 $\lambda = 1.9 \times 10^{-4} \text{ d}^{-1}$ case 2 $\lambda = 0$	
Distribution coefficient, k_d case 1 $k_d = 0.308 \text{ cm}^3/\text{g}$ case 2 $k_d = 0$	

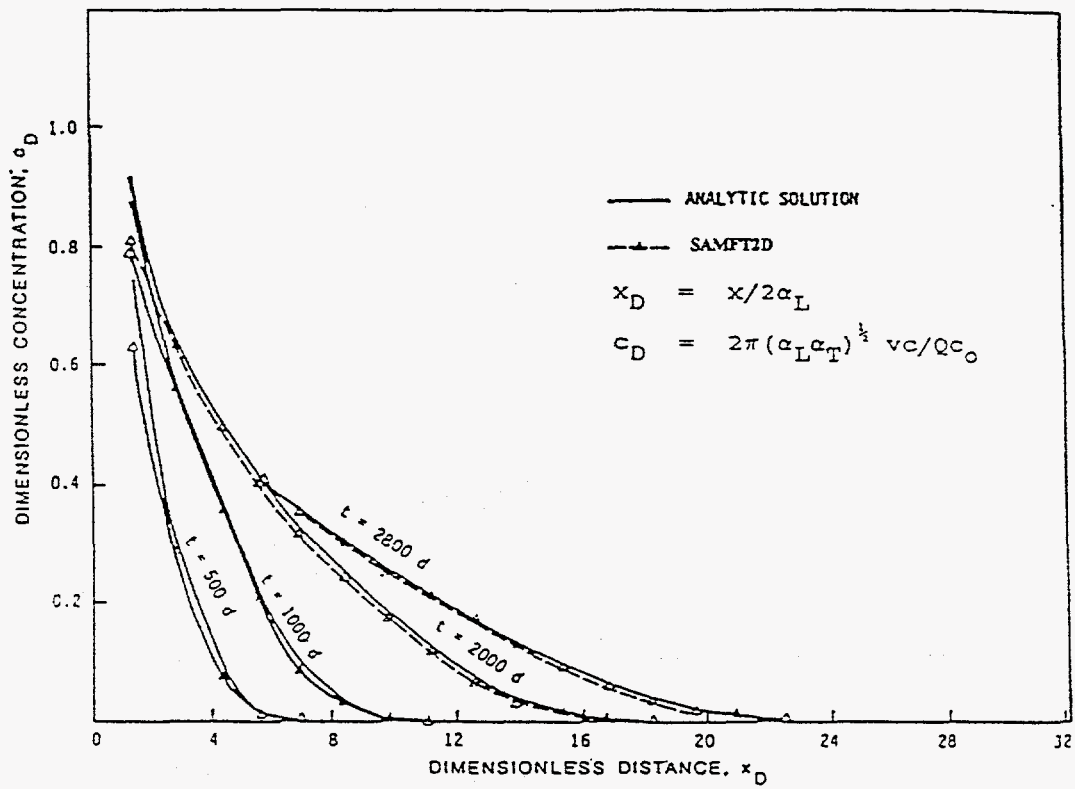


Figure 4.16. Simulated profiles of dimensionless concentration along the x-axis (case 1).

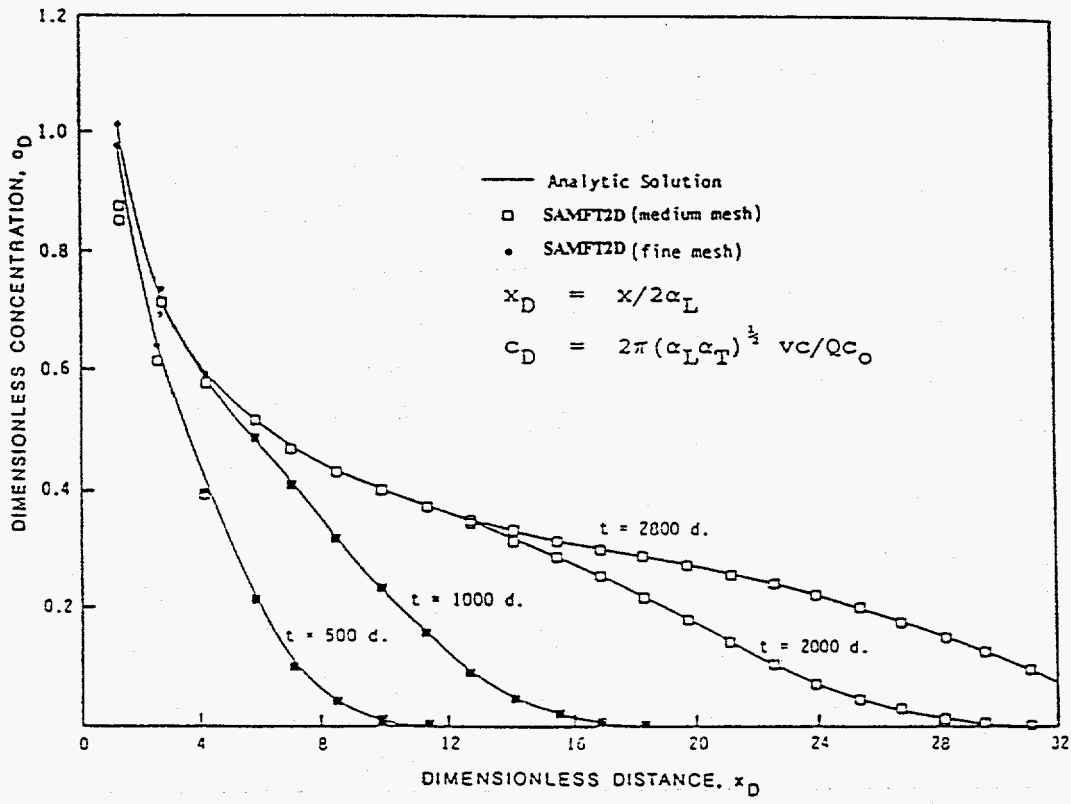


Figure 4.17. Simulated profiles of dimensionless concentration along the x-axis (case 2).



Figure 4.18. Simulated and observed plumes of hexavalent chromium.

4.3.4 Leachate Migration from a Landfill

This steady-state transport problem is associated with the steady-state variably saturated flow problem described in Section 4.2.4. It was selected to demonstrate another potential application of SAMFT2D in the investigation groundwater contamination due to land disposal of toxic waste. Shown in Figures 4.19a and 4.19b are the transport scenario modeled and a steady-state contaminant plume predicted by SAMFT2D using the flow field and water saturation distribution obtained from the related flow simulation. Note that the simulated plume exhibits limited lateral and vertical dispersion. Within the vadose zone, the concentration contours are tightly spaced and confined to narrow bands near the landfill boundary. The plume center line shows a significant dip in the saturated zone due to the effect of downward vertical groundwater flow components caused by a slight mounding of the water table.

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). Both the fluids and porous material were assumed to be incompressible, and capillary effects are ignored. The geometry and boundary conditions of the flow domain are shown in Figure 4.20. The system was initially saturated with water ($S_w = 0.2$) and NAPL ($S_n = 0.8$), water was injected with a constant injection rate at the inlet, $x=0$ from $t=0$. The flow cross-sectional area was 10 m^2 . On the outlet boundary, $x = 305\text{m}$, the pressures for the two fluids were kept to be at zero reference pressures.

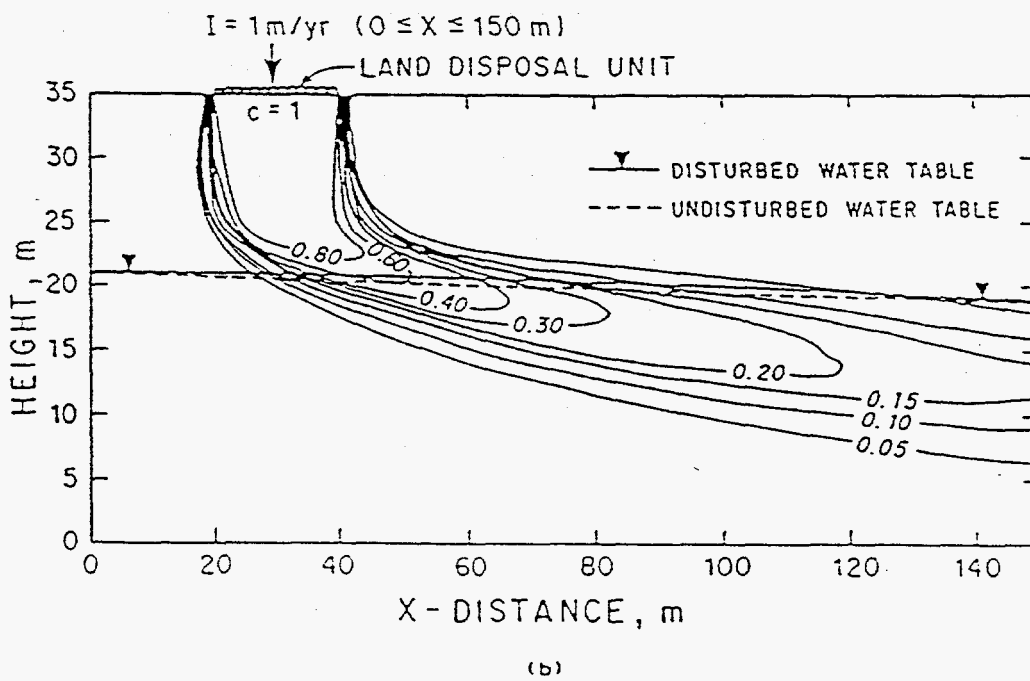
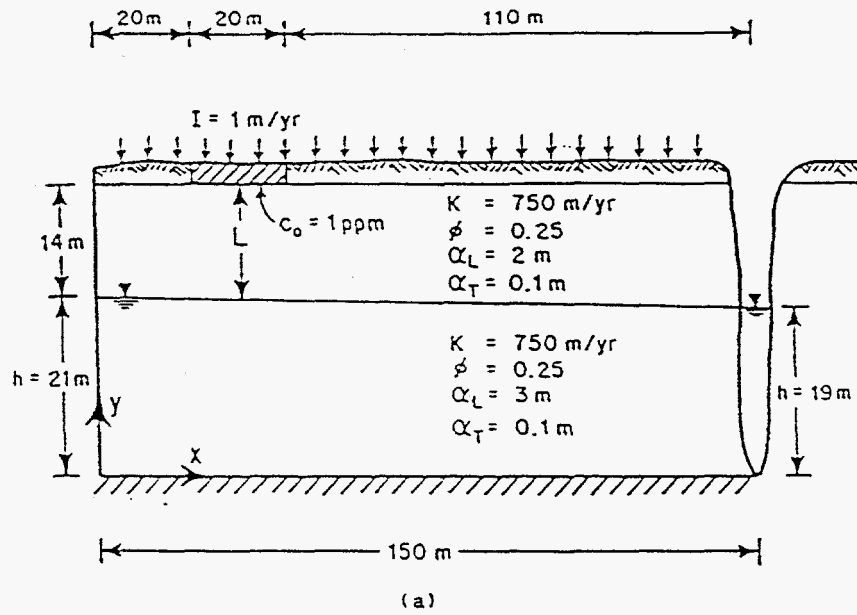


Figure 4.19. Problem description and simulation result for the scenario of leachate migration from a land disposal unit.

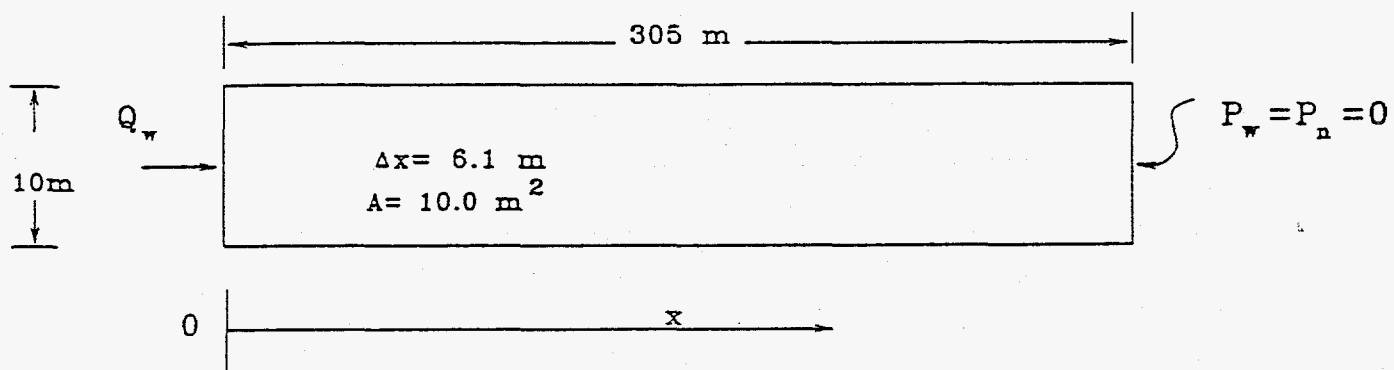


Figure 4.20. Geometry and boundary conditions used in the simulation of the Buckley-Leverett flow problem in a horizontal one-dimensional system.

The properties of formation and fluids are summarized in Table 4.6. Data used in this simulation were extracted from the work of Nilkuha and Huyakorn (1980). The relative permeability functions used are as follows:

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

and

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

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

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

$$\left. \begin{array}{l} k_{rw} = 1 \\ k_{rn} = 0 \end{array} \right\}$$

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

$$\left. \begin{array}{l} k_{rw} = 0 \\ k_{rn} = 1 \end{array} \right\}$$

The flow domain was discretized into 50 linear rectangular elements, and constant mesh spacings ($\Delta x = 6.1\text{m}$ and $\Delta y = 10\text{m}$) were used. The porous medium was assumed to be homogeneous with constant permeability and initial porosity, as given in Table 4.5. The simulation was performed for 60 time steps. The time step values were generated within the

Table 4.6 Porous medium and fluid properties used in the simulation of the Buckley-Leverett flow problem.

Parameter	Value
Permeability, k	$0.3 \times 10^{-12} \text{ m}^2$
Porosity, ϕ	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	$86.4 \text{ kg}/(\text{m-d})$
NAPL Viscosity, μ_n	$86.4 \text{ kg}/(\text{m-d})$
Water Injection Rate, Q_w	$0.13 \text{ m}^3/\text{d}$
Water Density, ρ_w	$1000 \text{ kg}/\text{m}^3$
NAPL Density, ρ_n	$1000 \text{ kg}/\text{m}^3$

code using the algorithm: $\Delta t_1 = 20$ d, $\Delta t_n = 1.2 \Delta t_{n-1} \leq 80$ d for $n = 2, 3, \dots, 60$. 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 SAMFT2D and the Buckley-Leverett analytical solution after 967 days of water injection is shown in Figure 4.21. Also included in the same figure is the corresponding block-centered 1-D finite difference solution from the SAMFT1D code documented by Wu, et al. (1991). As can be seen, the numerical results from both SAMFT1D and SAMFT2D 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, et al. (1990).

4.4.2 Vertical Two-Phase Flow without Capillary Effect

This second test problem concerns two-phase flow through a vertical sand formation column. If capillary effects are negligible, the Buckley-Leverett type analytical solution is also available in the literature (Wu, et al., 1990) to examine the numerical solutions. Geometry and boundary conditions for this test are described in Figure 4.22. In this case, all of fluid and formation properties, flow system dimensions, initial conditions, and constitutive equations for relative permeability are almost identical to those in the previous test problem. The only changes made are: 1) NAPL density is $\rho_n = 864$ kg/m³, 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.

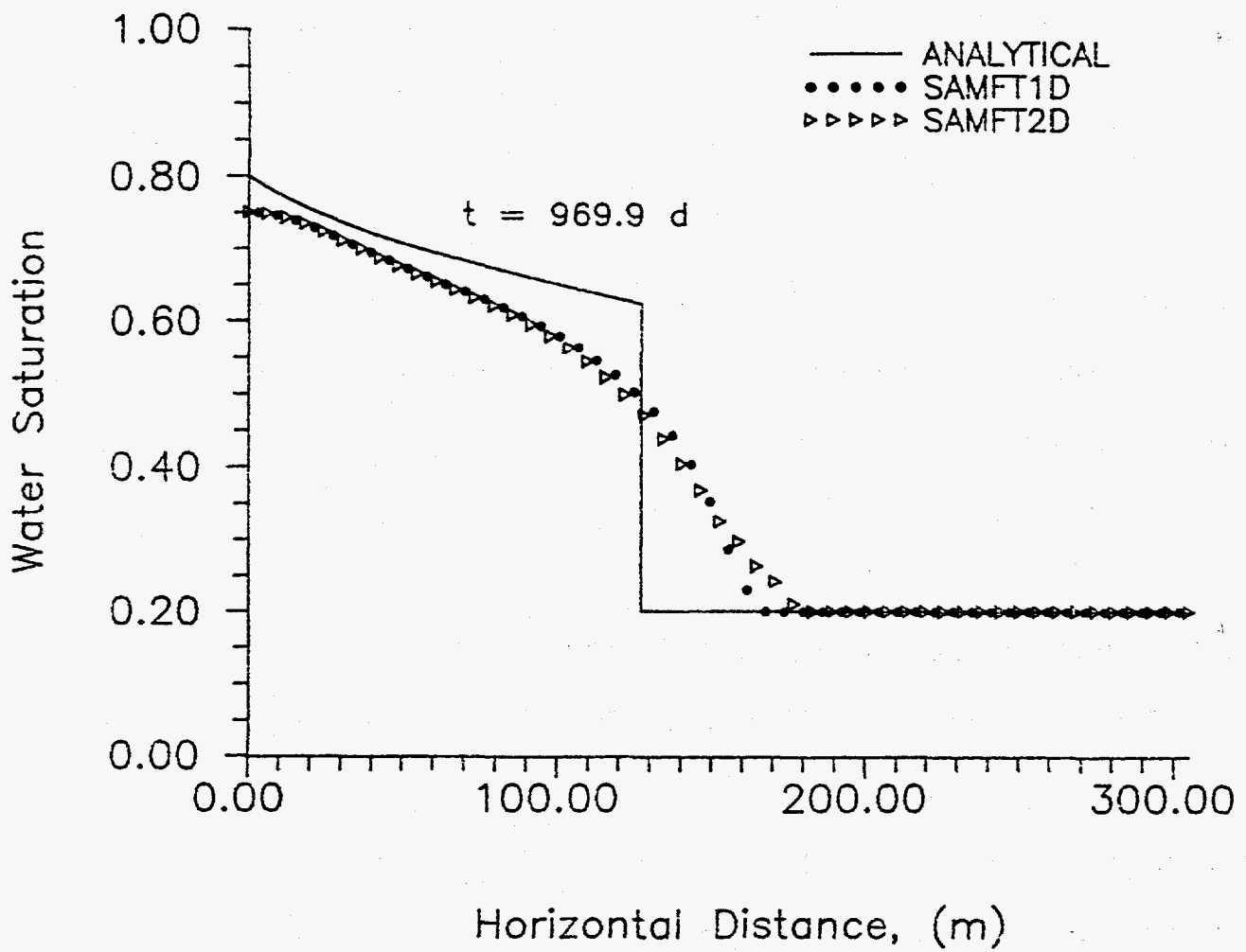


Figure 4.21. Comparison of water saturation profiles calculated from analytical and numerical solutions for horizontal two-phase water and NAPL flow.

As shown in Figure 4.22, the flow system was subjected to water flux at the top, and constant pressures at the bottom. The same grids and time-steps generation or reduction options described in section 4.4.1 were used for this case. Computed water saturation after 900 days of water injection by SAMFT2D and a comparison with the analytical solution and numerical result obtained using the SAMFT1D one-dimensional block-centered finite difference code are shown in Figure 4.23. As can be seen, there is good agreement between the numerical and analytical solutions.

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 difficult to represent because NAPL flux reduces to zero under buoyancy force from water. However, the numerical solution, as shown in Figure 4.23, 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 Vertical Two-Phase Flow in a Three-Phase System

This problem was designed to test the capability of SAMFT2D to handle immiscible fluid flow within and below the unsaturated zone including effects of gravity and capillary pressure. In this case, the air phase was treated as a passive phase, and the pressure in the air phase was assumed to be atmospheric. The flow domain and conditions are shown in Figure 4.24. Initially, the 5-meter soil column contained both saturated and unsaturated zones with initial

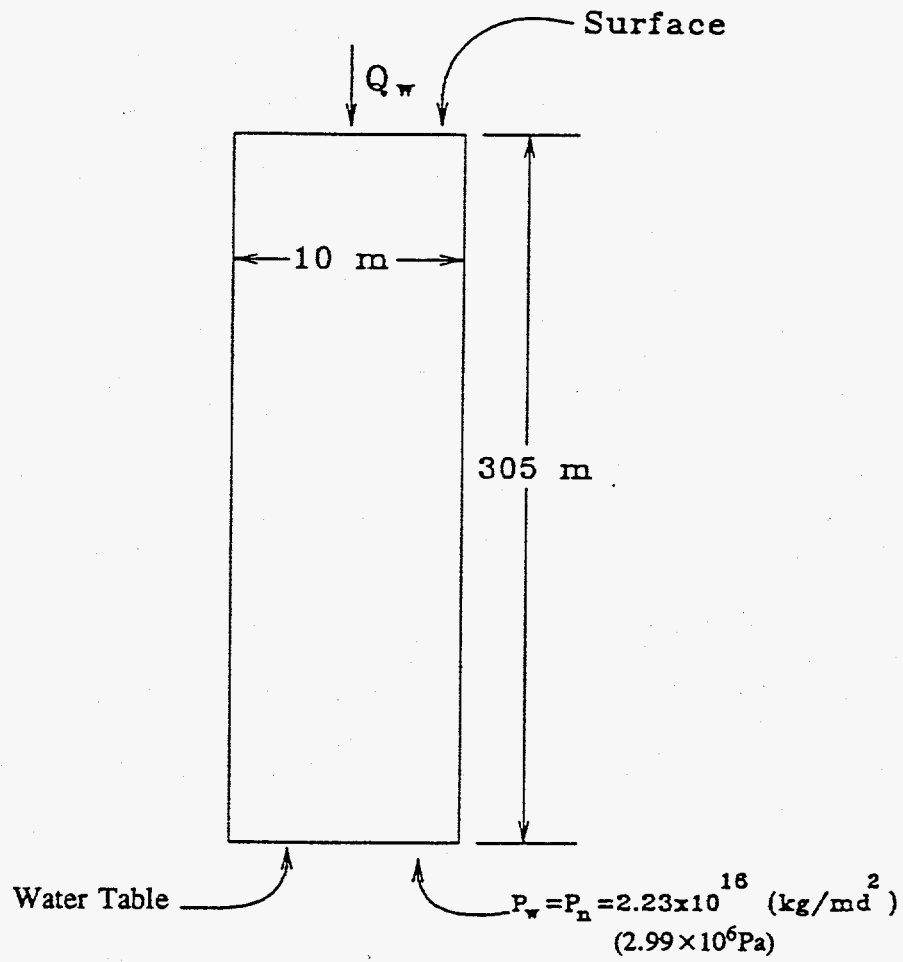


Figure 4.22. Geometry and boundary conditions used in the simulation of the two-phase flow problem in a vertical one-dimensional system.

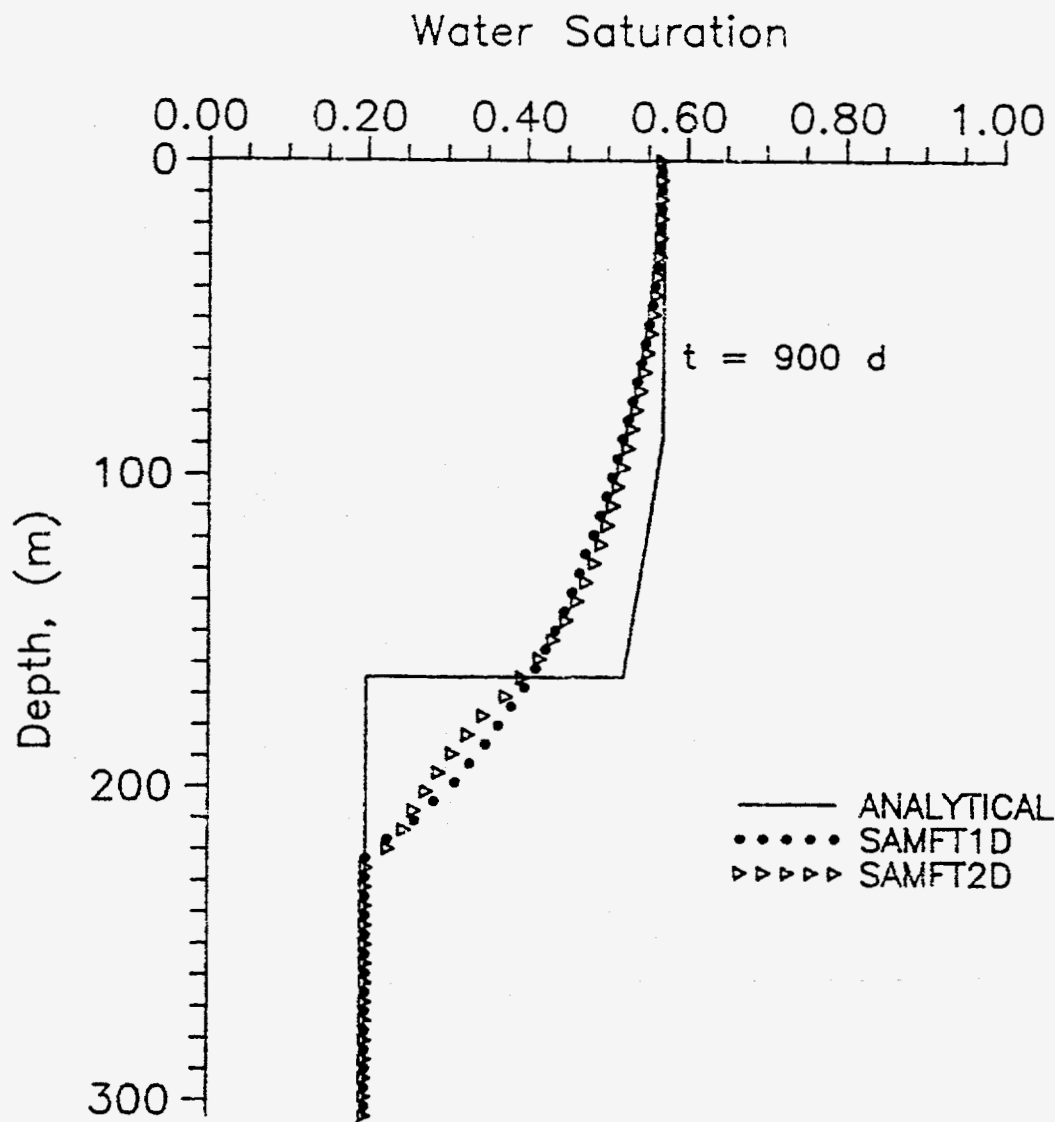


Figure 4.23. Comparison of water saturation profiles calculated from analytical and numerical solution for vertical two-phase water and NAPL flow.

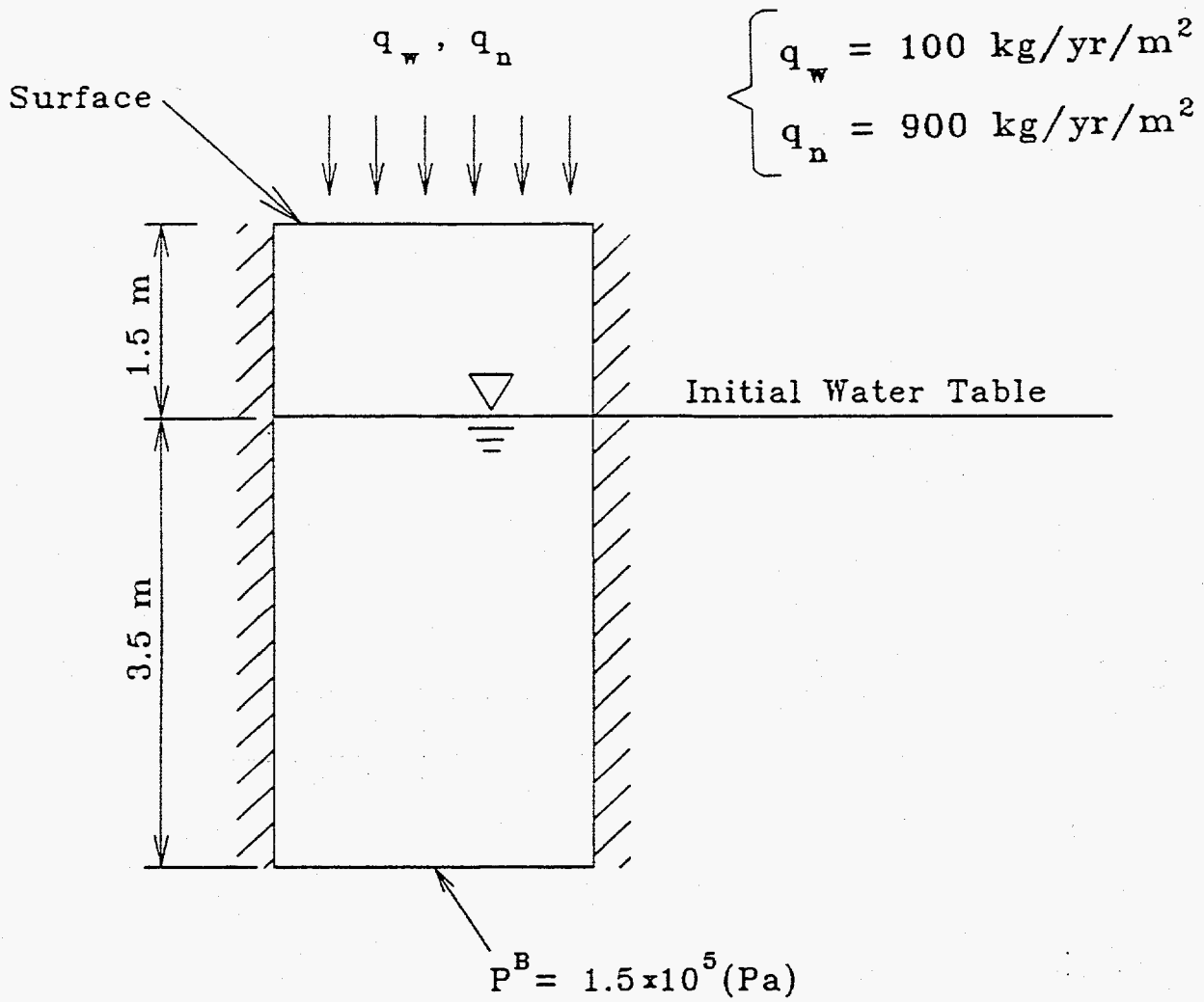


Figure 4.24. Geometry and boundary conditions in the simulation vertical two-phase flow in a three-phase system.

water table 1.5 meter below the surface. The surface boundary was subjected to simultaneous injection of water and NAPL, and the bottom boundary was subjected to a constant pressure. The physical parameters for the simulation are given in Table 4.7.

The one-dimensional flow domain was discretized into 20 elements with constant mesh spacings ($\Delta x = 1\text{m}$, $\Delta y = 0.25\text{m}$). The initial condition generated by the code is given in Table 4.8, and relative permeability and capillary pressure data taken from Faust (1985) and (Forsyth, 1990) are shown in Table 4.9. The simulation was performed for 60 time steps. The time steps were generated by the code using the scheme described in Chapter 3.

In order to verify the computational modules of SAMFT2D for modeling two-phase fluid flow under three-phase conditions, the simulation results of SAMFT2D were compared with the results from SAMFT1D and from the three-dimensional numerical model (NAPL3D) of Forsyth (1990). The comparison of NAPL and water saturations from SAMFT2D, SAMFT1D and NAPL3D at five time values from 10 to 500 days are shown in Figures 4.25 and 4.26, respectively. As can be seen, the numerical solutions from all the three codes are in excellent agreement.

4.4.4 Vertical Three-Phase Flow

This problem was designed to test the SAMFT2D 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 4.4.4. Also, the same parameters, initial conditions (Table 4.8), and relative permeability and capillary pressure data (Table 4.9) were used in this case. However, one additional surface boundary condition was needed for the air flow equation, and a zero flux

Table 4.7 Parameter values used in the simulation of two-phase flow in a three-phase system.

Parameter	Value
Permeability, k	$1 \times 10^{-12} \text{ m}^2$
Porosity, ϕ	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^0	$1,000 \text{ kg/m}^3$
Initial NAPL Density, ρ_n^0	950 kg/m^3
Water Viscosity, μ_w	$1 \times 10^{-3} \text{ Pa}\cdot\text{s}$
NAPL Viscosity, μ_n	$1 \times 10^{-3} \text{ Pa}\cdot\text{s}$
Water Compressibility, β_w	$4.3 \times 10^{-9} \text{ Pa}^{-1}$
NAPL Compressibility, β_n	$3.0 \times 10^{-9} \text{ Pa}^{-1}$
Porous Medium Compressibility, β_s	10^{-10} Pa^{-1}
Water Injection Rate, q_w	100 kg/yr/m^2
NAPL Injection Rate, q_n	900 kg/yr/m^2
Bottom Pressure, p^B	$1.5 \times 10^5 \text{ Pa}$

Table 4.8 Initial Condition Used in the Simulation of Two-Phase Flow in a Three-Phase System.

<u>Depth</u> (m)	<u>P_n</u> N/m ² (Pa)	<u>S_w</u>	<u>S_n</u>
0.125	0.9850E+05	0.8500E+00	0.0
0.375	0.9877E+05	0.8773E+00	0.0
0.625	0.9905E+05	0.9045E+00	0.0
0.875	0.9932E+05	0.9318E+00	0.0
1.125	0.9959E+05	0.9591E+00	0.0
1.375	0.9986E+05	0.9864E+00	0.0
1.625	0.1012E+06	0.1000E+01	0.0
1.875	0.1037E+06	0.1000E+01	0.0
2.125	0.1061E+06	0.1000E+01	0.0
2.375	0.1086E+06	0.1000E+01	0.0
2.625	0.1110E+06	0.1000E+01	0.0
2.875	0.1135E+06	0.1000E+01	0.0
3.125	0.1159E+06	0.1000E+01	0.0
3.375	0.1184E+06	0.1000E+01	0.0
3.625	0.1208E+06	0.1000E+01	0.0
3.875	0.1233E+06	0.1000E+01	0.0
4.125	0.1257E+06	0.1000E+01	0.0
4.375	0.1282E+06	0.1000E+01	0.0
4.625	0.1306E+06	0.1000E+01	0.0
4.875	0.1331E+06	0.1000E+01	0.0

Table 4.9 Relative permeability and capillary pressure data used in the simulation of two-phase flow in a three-phase system.

Two-Phase Water - NAPL (wn) System				
S_w	k_{rw}	k_{rn}^{wn}	$P_{cnw}(\text{Pa})$	
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	0.0	

Two-Phase NAPL-air (na) and air-water Systems				
S_a	k_{ra}	k_{rn}^n	$P_{can}(\text{Pa})$	$P_{caw}(\text{Pa})$
0.00	0.00	0.680	0.00	0.00
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

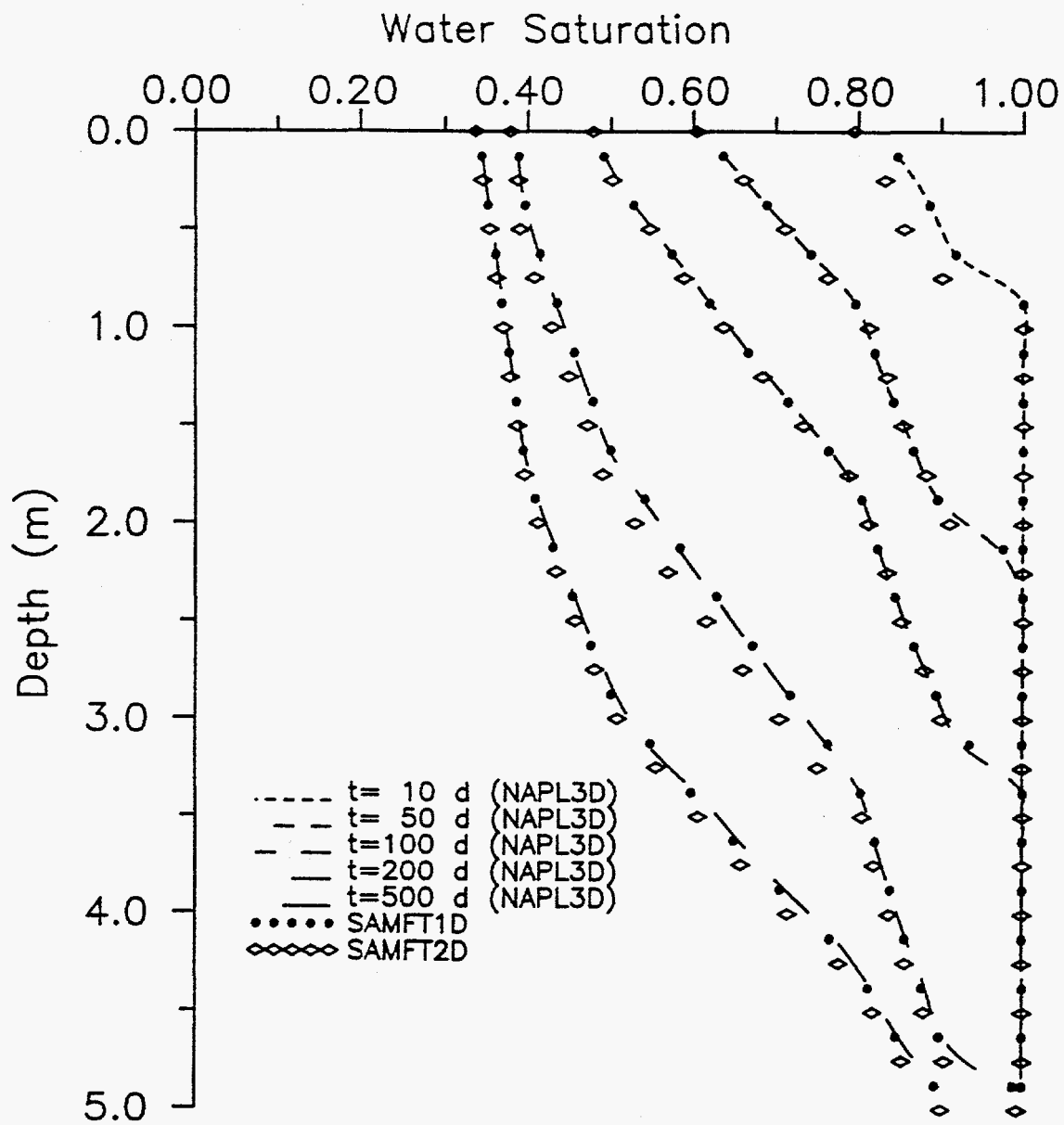


Figure 4.25. Comparison of water saturations calculated from SAMFT2D, SAMFT1D and NAPL3D (Forsyth, 1990) for two-phase flow under three-phase condition.

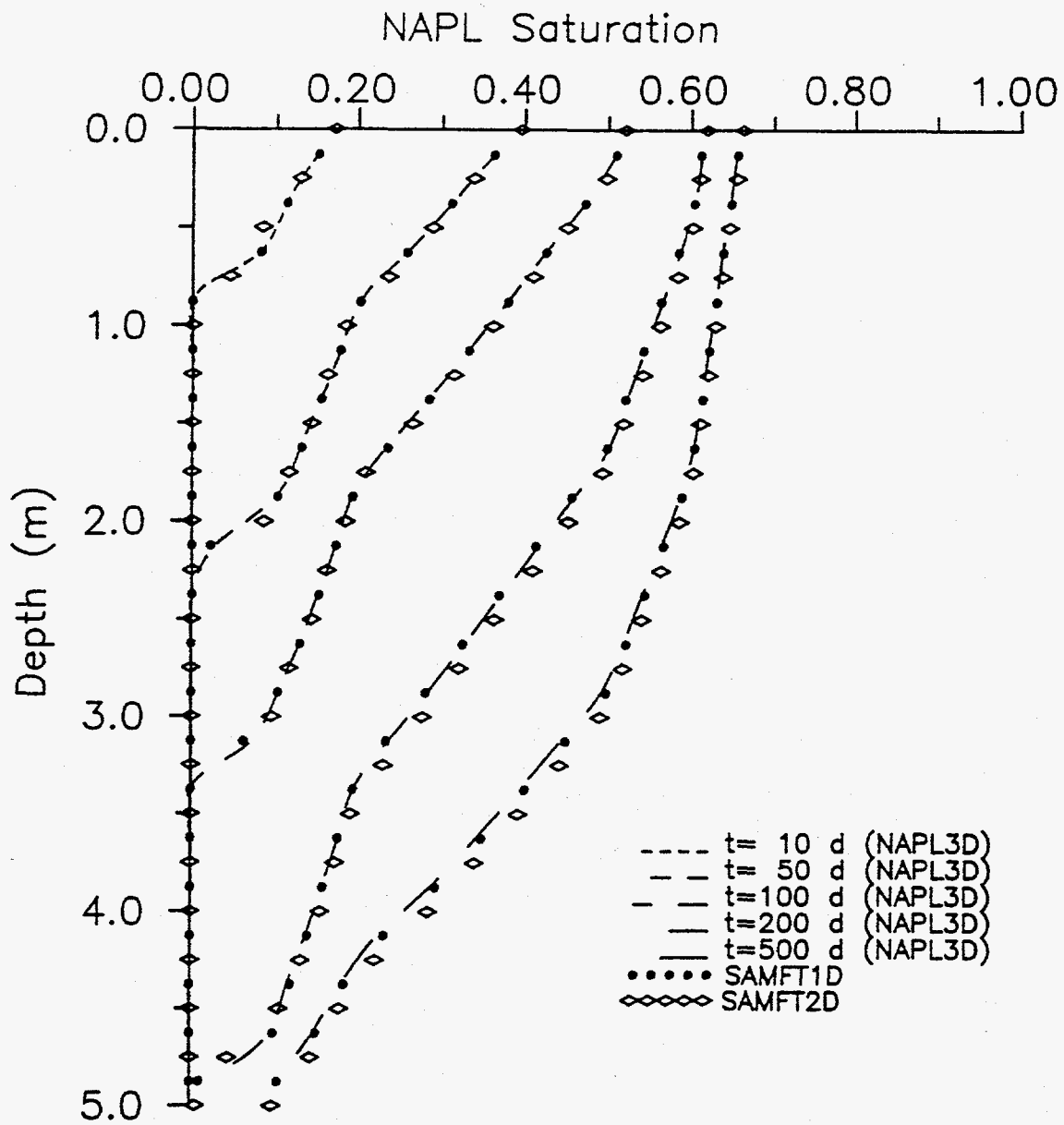


Figure 4.26. Comparison of NAPL saturations calculated from SAMFT2D, SAMFT1D and NAPL3D (Forsyth, 1990) for two-phase flow under three-phase condition.

condition was used in this case, i.e., no air was allowed to cross the surface boundary. The automatic time stepping algorithm was also used in this simulation to compute and update time step values.

The simulation results obtained from SAMFT2D were checked against SAMFT1D and a three-dimensional compositional model by Forsyth and Shao (1991). The comparison of NAPL and water saturations from the three codes is given in Figures 4.27 and 4.28, respectively. The agreement between the simulation results as shown in both figures from the three-phase flow and compositional codes is good. 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 SAMFT2D and SAMFT1D. The compositional model treats the water as a component which exists in both the water and air phases as well. In this case, there is 10% water in the air phase. After a few grid blocks from the surface, the results obtained from the three models are more closely matching each other as can be seen in Figures 4.27 and 4.28. 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.

4.4.5 Two-Dimensional Migration of NAPL in a Variably Saturated Groundwater System

This example was selected to verify SAMFT2D for a situation concerning two-dimensional migration of NAPL in a surficial formation having both the unsaturated and saturated zones. The problem considered corresponds to that solved by Faust (1985). Two cases involving LNAPL with density less than water and DNAPL with density greater than water were simulated.

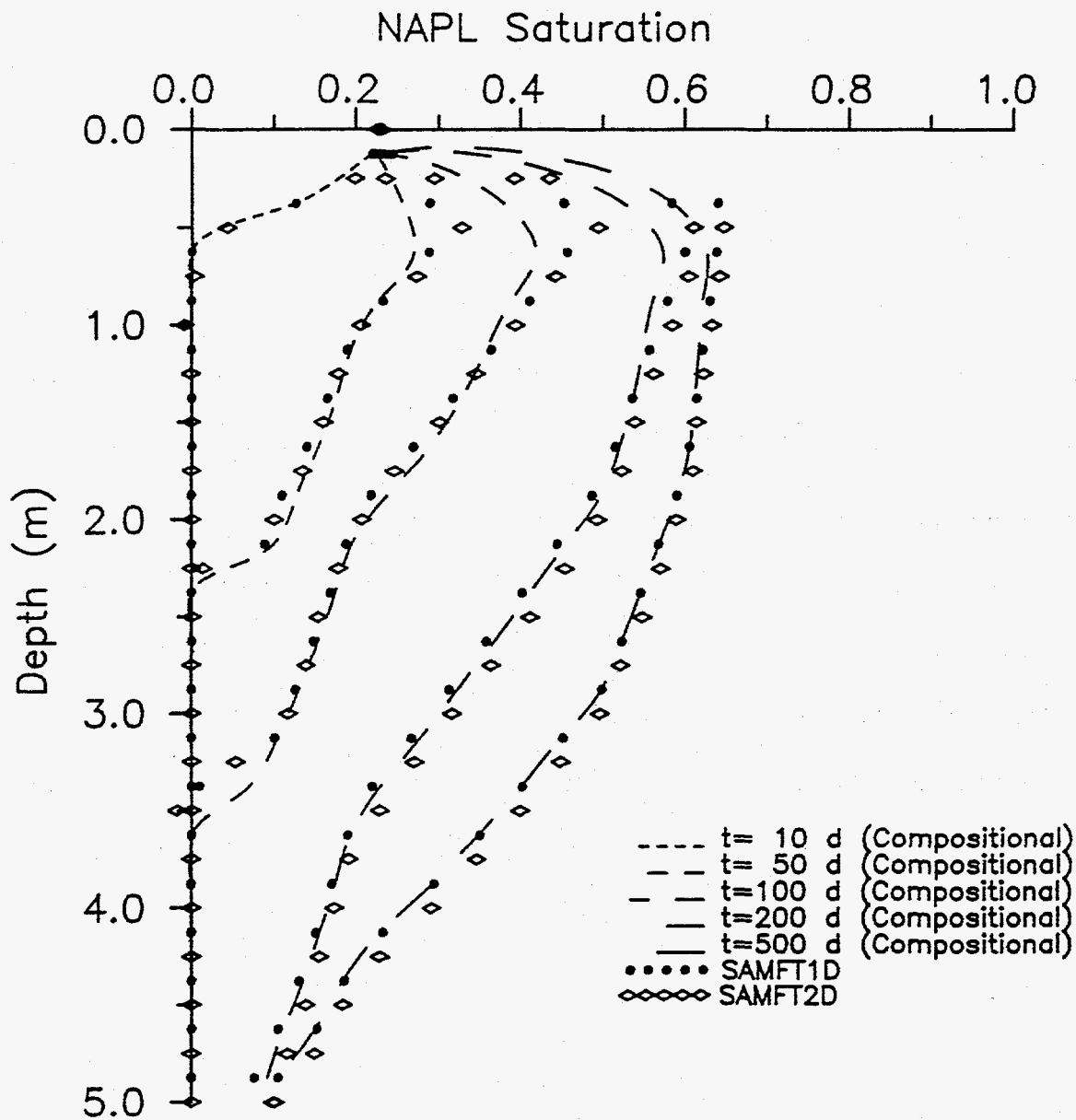


Figure 4.27. Comparison of NAPL saturations calculated from SAMFT2D, SAMFT1D and compositional model (Forsyth and Shao, 1991).

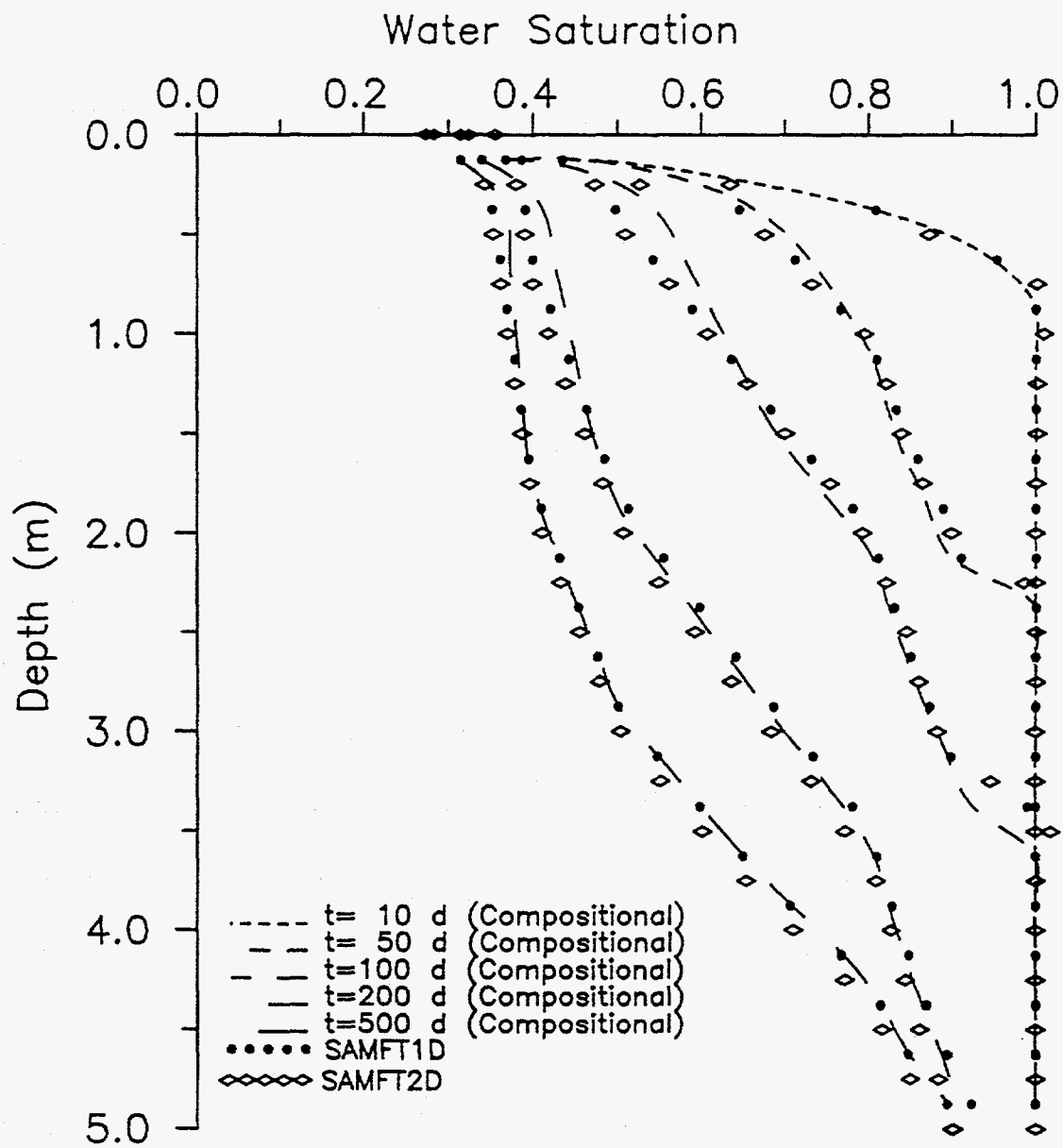


Figure 4.28. Comparison of water saturations calculated from SAMFT1D and compositional model (Forsyth and Shao, 1991).

The modeled flow system (Figure 4.29) consists of a surficial unit 5m thick and subjected to a uniform infiltration rate of 0.1 m/yr (100 kg/yr/m²). The NAPL source is located at the left-hand corner of the flow domain and its leakage rate was assumed to be 900 kg/yr. The surficial unit has a shallow water table (1.5m deep) and is underlain by a draining aquifer. The vertical boundaries of the modeled domain were treated as impermeable and the bottom boundary was prescribed constant absolute pressure values of $\tilde{p}_a = 1.3185 \times 10^5 \text{ N/m}^2$ and $\tilde{p}_w = 1.2495 \times 10^5 \text{ N/m}^2$ (Pa).

A summary of physical parameter values used in the simulation is provided in Table 4.10. The initial conditions and tabulated constitutive relations are given in Tables 4.11 and 4.12, respectively. Note that the initial pressure values in Table 4.11 are absolute values rather than gauge (or relative) values used by Faust (1985). To be consistent with Faust's modeling assumption we evaluated p_{caw} as the sum of $p_{can} + p_{cnw}$.

The SAMFT2D code was run using the two active-phase formulation and a rectangular grid consisting of 120 elements and 147 nodes. The nodal spacings in the horizontal x-direction (Δx_i , $i=1, 6$) were 1, 1.41, 2, 2.83, 4 and 5.66 m. A constant nodal spacing of $\Delta y = 0.25$ was used in the vertical direction. The time step parameter values used were $\Delta t_1 = 10,000 \text{ s}$, and $\Delta t_{max} = 864,000 \text{ s}$ (10 days). The automatic time stepping algorithm was also used to compute and update time step values.

For the first case of LNAPL with density of 950 kg/m³, a contour plot of saturations is shown in Figure 4.29 for $t = 372$ days. As expected, the LNAPL plume has a lenticular shape and the LNAPL mass floats on the water table. The LNAPL saturation contours obtained by

Table 4.10 Physical parameter values used in the analysis of problem 4.4.6.

Parameter	Value
Permeability, k	$1 \times 10^{-12} \text{ m}^2$
Porosity, Θ	0.3
Water Density, ρ_w	$1,000 \text{ kg/m}^3$
Light NAPL Density, ρ_n	950 kg/m^3
Dense NAPL Density, ρ_n	$1,200 \text{ kg/m}^3$
Water Viscosity, μ_w	$1 \times 10^{-3} \text{ Pa}\cdot\text{s}$
NAPL Viscosity, μ_n	$1 \times 10^{-3} \text{ Pa}\cdot\text{s}$
Water Injection Infiltration Rate, q_w	100 kg/yr/m^2
Total NAPL Injection Rate, Q_n	900 kg/yr
Bottom Water Pressure, P_w	$1.2495 \times 10^5 \text{ Pa}$
Bottom NAPL Pressure, P_n	$1.3185 \times 10^5 \text{ Pa}$

Table 4.11 Initial conditions used in the analysis of problem 4.4.6.

Depth (m)	P_n N/m ² (Pa)	S_w	S_n
0.125	0.761237E+05	0.0	0.8500E+06
0.375	0.783879E+05	0.0	0.8700E+00
0.625	0.817841E+05	0.0	0.9000E+00
0.875	0.846143E+05	0.0	0.9250E+00
1.125	0.874446E+05	0.0	0.9500E+00
1.375	0.902748E+05	0.0	0.9750E+00
1.625	0.943308E+05	0.0	0.1000E+01
1.875	0.967825E+05	0.0	0.1000E+01
2.125	0.992341E+05	0.0	0.1000E+01
2.375	0.101686E+06	0.0	0.1000E+01
2.625	0.104137E+06	0.0	0.1000E+01
2.875	0.106589E+06	0.0	0.1000E+01
3.125	0.109041E+06	0.0	0.1000E+01
3.375	0.111492E+06	0.0	0.1000E+01
3.625	0.113944E+06	0.0	0.1000E+01
3.875	0.116396E+06	0.0	0.1000E+01
4.125	0.118847E+06	0.0	0.1000E+01
4.375	0.121299E+06	0.0	0.1000E+01
4.625	0.123751E+06	0.0	0.1000E+01
4.875	0.126202E+06	0.0	0.1000E+01

Table 4.12. Relative permeability and capillary pressure data used in the analysis of problem 4.4.6.

Two-Phase Water-NAPL System				
S_w	k_{rw}	k_{rn}^{wn}	P_{cnw} (Pa)	
0.2000E+00	0.0000E+00	0.6800E+00	0.1034E+06	
0.3000E+00	0.4000E-01	0.5500E+00	0.2758E+05	
0.4000E+00	0.1000E+00	0.4300E+00	0.1034E+05	
0.5000E+00	0.1800E+00	0.3100E+00	0.7585E+04	
0.6000E+00	0.3000E+00	0.2000E+00	0.7447E+04	
0.7000E+00	0.4400E+00	0.1200E+00	0.7309E+04	
0.8000E+00	0.6000E+00	0.5000E-01	0.7171E+04	
0.9000E+00	0.8000E+00	0.0000E+00	0.7033E+04	
0.1000E+01	0.1000E+01	0.0000E+00	0.6895E+04	

Two-Phase NAPL - Air and air-water Systems				
S_a	k_{ra}	k_{rn}^{na}	P_{can} (Pa)	P_{caw} (Pa)
0.0000E+00	0.0000E+00	0.6800E+00	0.0000E+00	0.6895E+04
0.6800E+00	0.6800E+00	0.0000E+00	0.6664E+05	0.8388E+05
0.8000E+00	0.8000E+00	0.0000E+00	0.7710E+05	0.1805E+06

Elapsed Time = 372 days

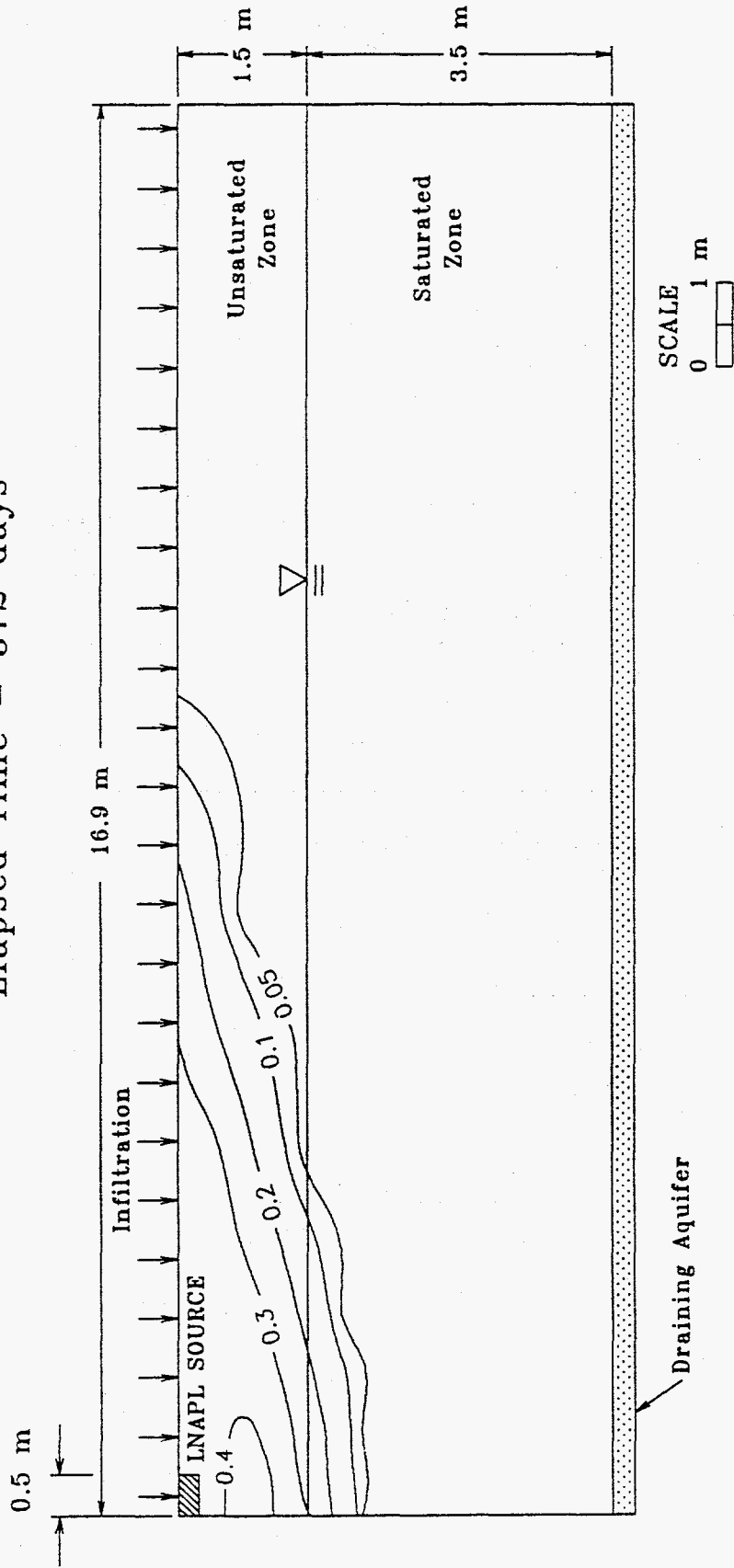


Figure 4.29. Flow system and simulated contours of LNAPL saturations for problem 4.4.6 (case 1).
4-57

SAMFT2D are in excellent agreement with the corresponding contours determined by Faust's model for $t = 1.07$ years.

For the second case of DNAPL with density of 1200 kg/m^3 , the numerical solution given by SAMFT2D is shown in Figure 4.30 for $t = 427$ days. In this case, the DNAPL mass sinks and exits the modeled flow system through the draining aquifer. The DNAPL saturation contour obtained by SAMFT2D are also in excellent agreement with the corresponding plot in Faust (1985) for $t = 1.16$ years.

4.4.6 Two-Dimensional Migration of LNAPL in a Fully Saturated Groundwater System

This example was selected to demonstrate an application of the two-phase flow module of SAMFT2D for a situation concerning NAPL migration in a fully saturated groundwater system. The flow domain was kept essentially the same as that for problem 4.4.5 but with the water table located at the top and without recharge. The physical parameter values and relative permeability and capillary pressure data are as given in Tables 4.10 and 4.12, respectively. The LNAPL leakage rate was assumed to be 1535 kg/yr . Initially, the system was in hydrostatic equilibrium and free of contamination. The vertical boundaries of the domain were treated as impermeable and the bottom boundary was prescribed constant value of $\tilde{p}_n = \tilde{p}_w = 1.5 \times 10^5 \text{ N/m}^2$. The flow domain was discretized using the same grid as before. The time step parameter values used were $\Delta t_{\text{max}} = 864,000 \text{ s}$ (10 days). Contour plots of LNAPL saturations obtained for $t = 292 \text{ d}$ and $t = 615 \text{ d}$ are shown in Figures 4.31 and 4.32, respectively. At the later time value, the enlarged LNAPL plume has reached the right hand impermeable boundary.

Elapsed Time = 427 days

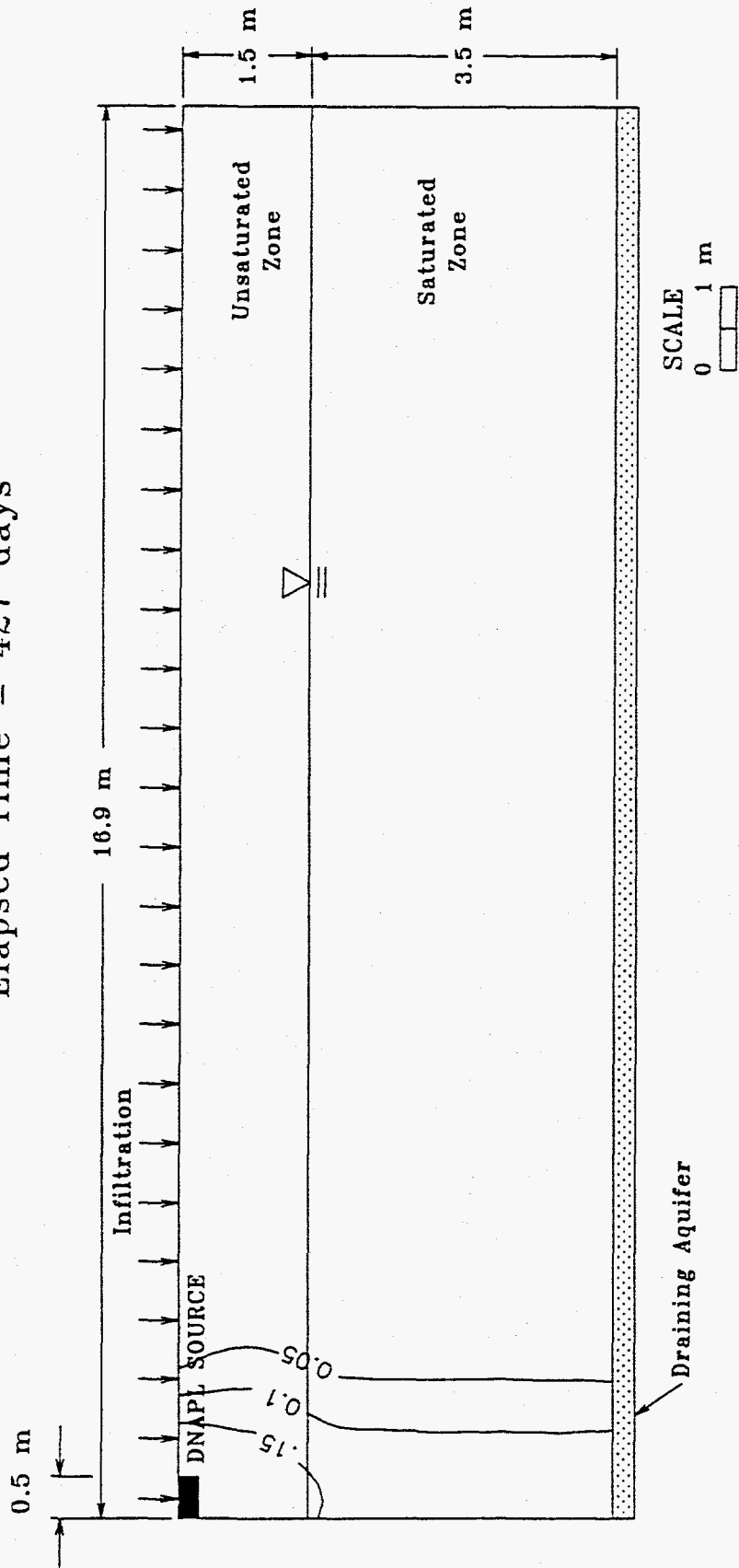


Figure 4.30. Flow system and simulated contours of DNAPL saturations for problem 4.4.6 (case 2).
4-59

Elapsed Time = 292 days

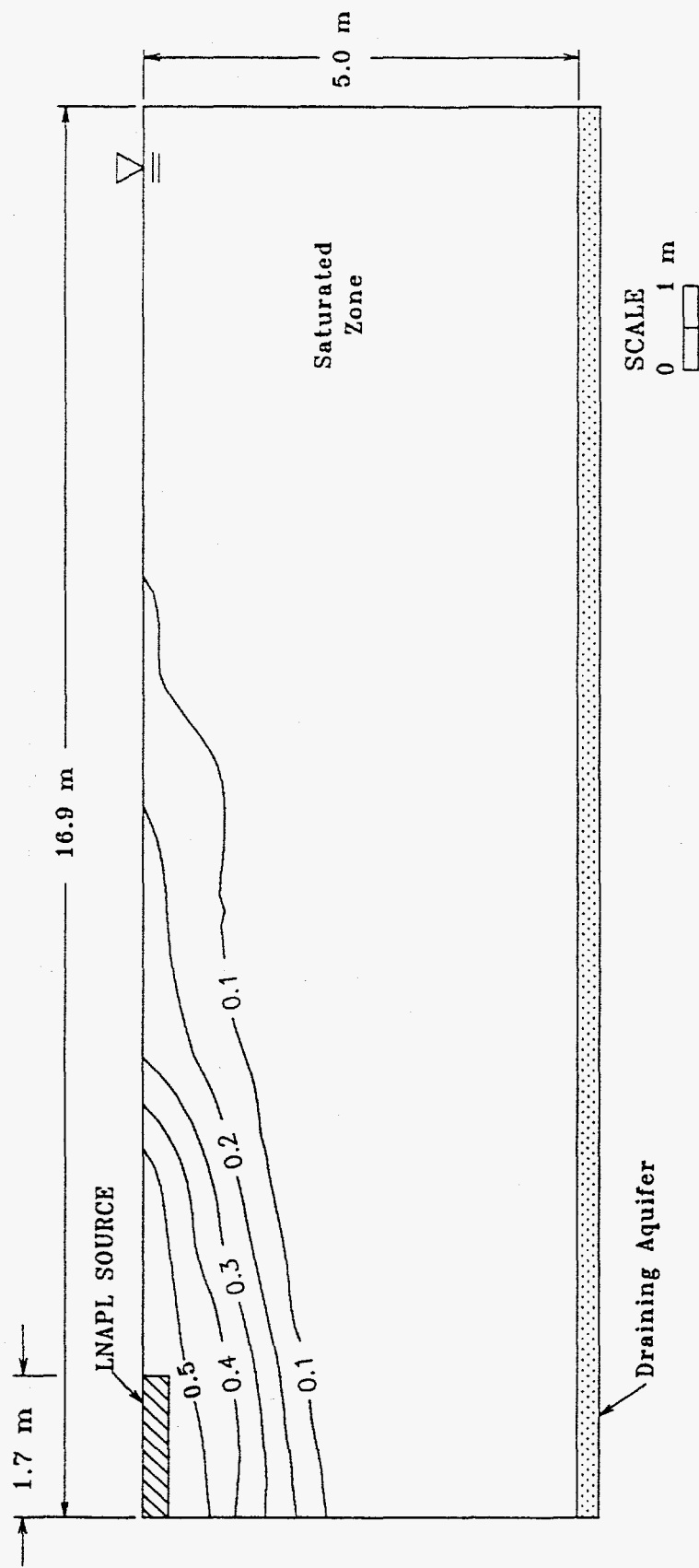


Figure 4.31. Flow system and simulated contours of LNAPL saturations for problem 4.4.7 ($t = 292$ d).
4-60

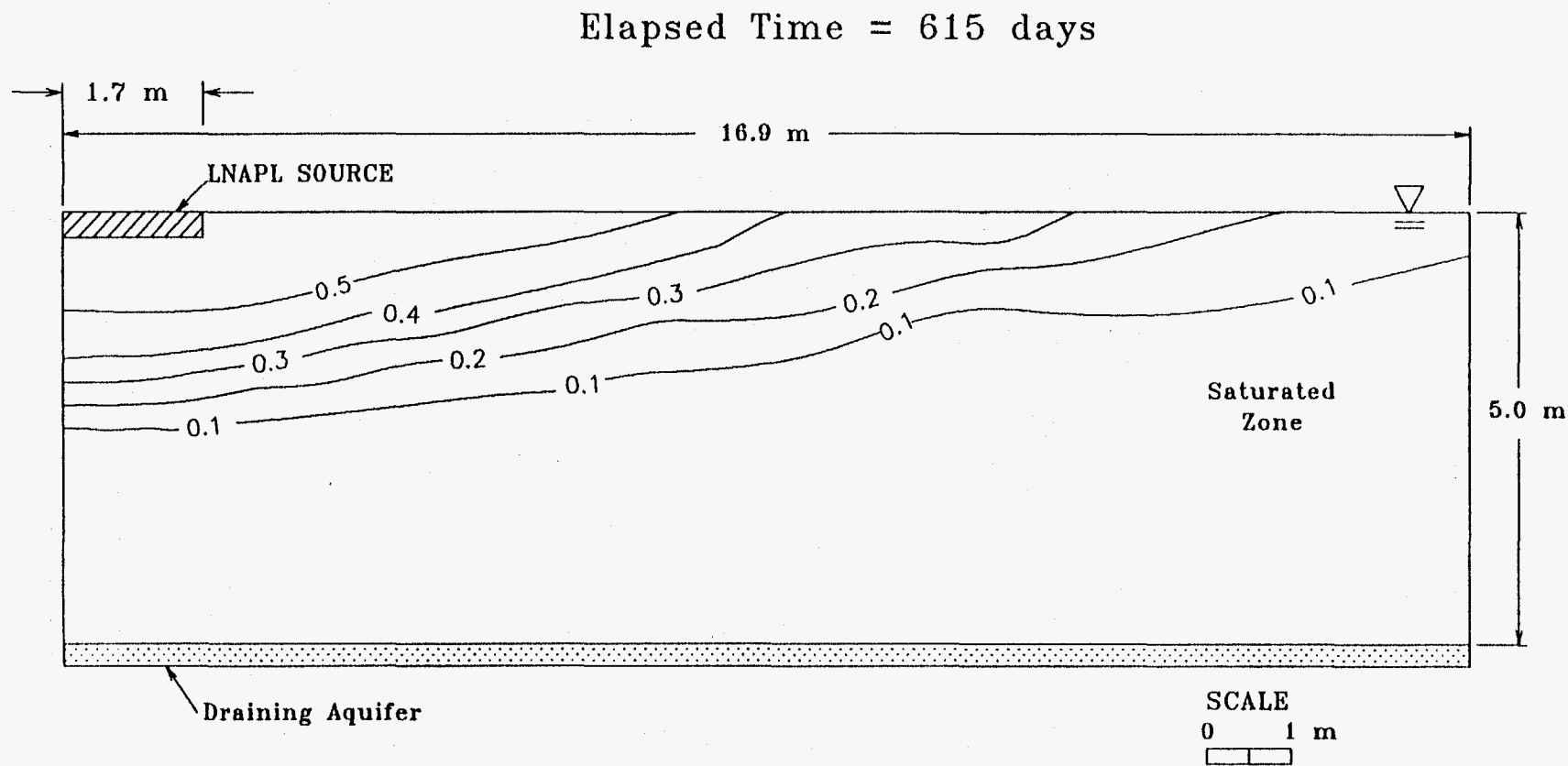


Figure 4.32. Flow system and simulated contours of LNAPL saturations for problem 4.4.7 ($t = 615$ d).
4-61

4.5 MULTIPHASE TRANSPORT PROBLEMS

4.5.1 One-Dimensional Transport of Dissolved Mass of LNAPL Spill

This example was selected to demonstrate an application of 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 4.33. The domain was discretized into 20 rectangular elements with constant nodal spacings ($\Delta x = 1$ m, $\Delta y = 0.50$ m). The surface boundary was subjected to water and LNAPL injection at $t = 0$. 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. The relative permeability and capillary pressure data is as given for the flow problem in Section 4.4.4. 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 4.34.

Following the flow simulation, the single-component transport simulation was performed with the stagnant LNAPL mass treated as "the precipitated mass (see Section 2.3.2)." The

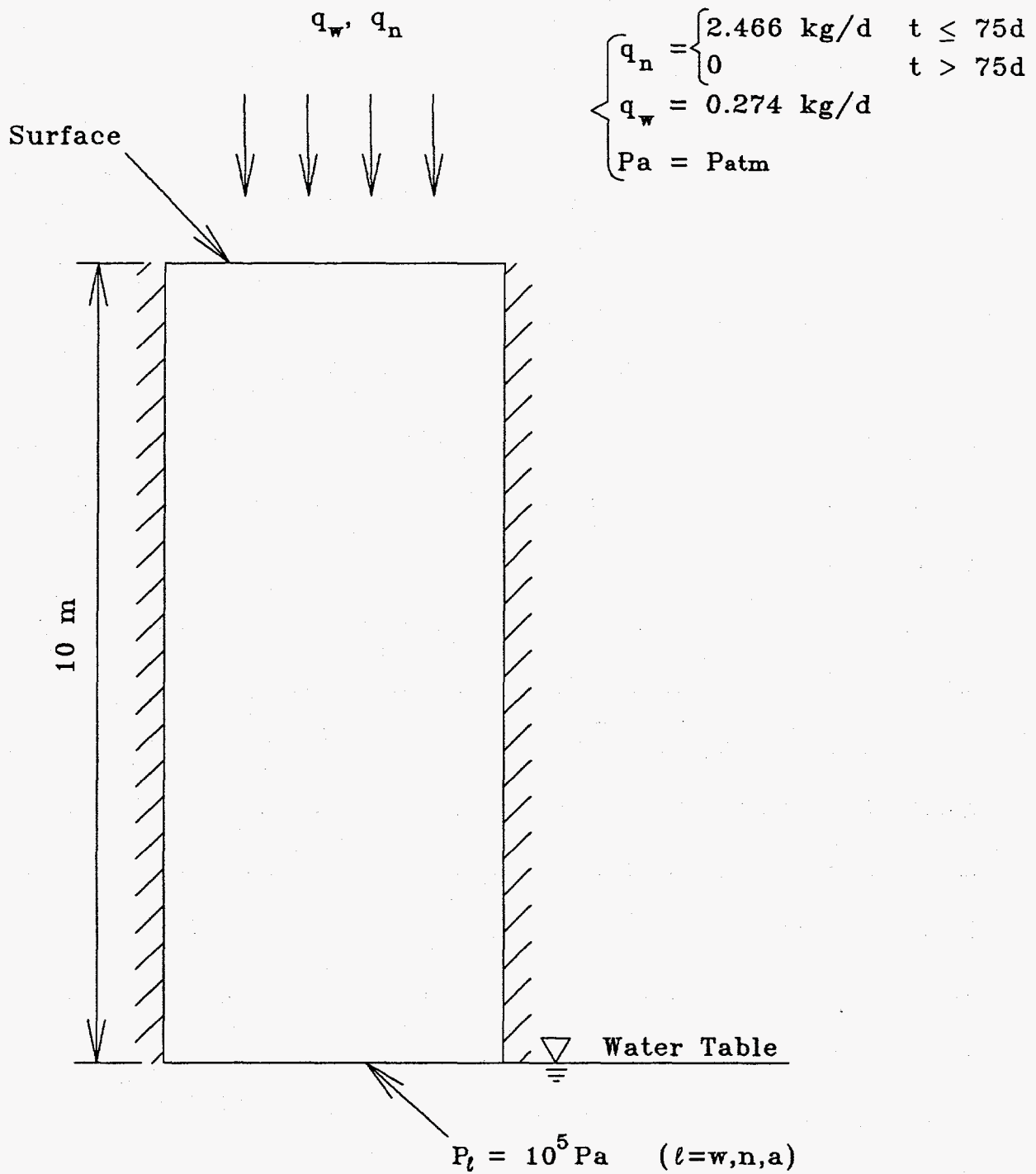


Figure 4.33. Geometry and boundary conditions used in the three-phase flow simulation with pulse release of NAPL on the surface.

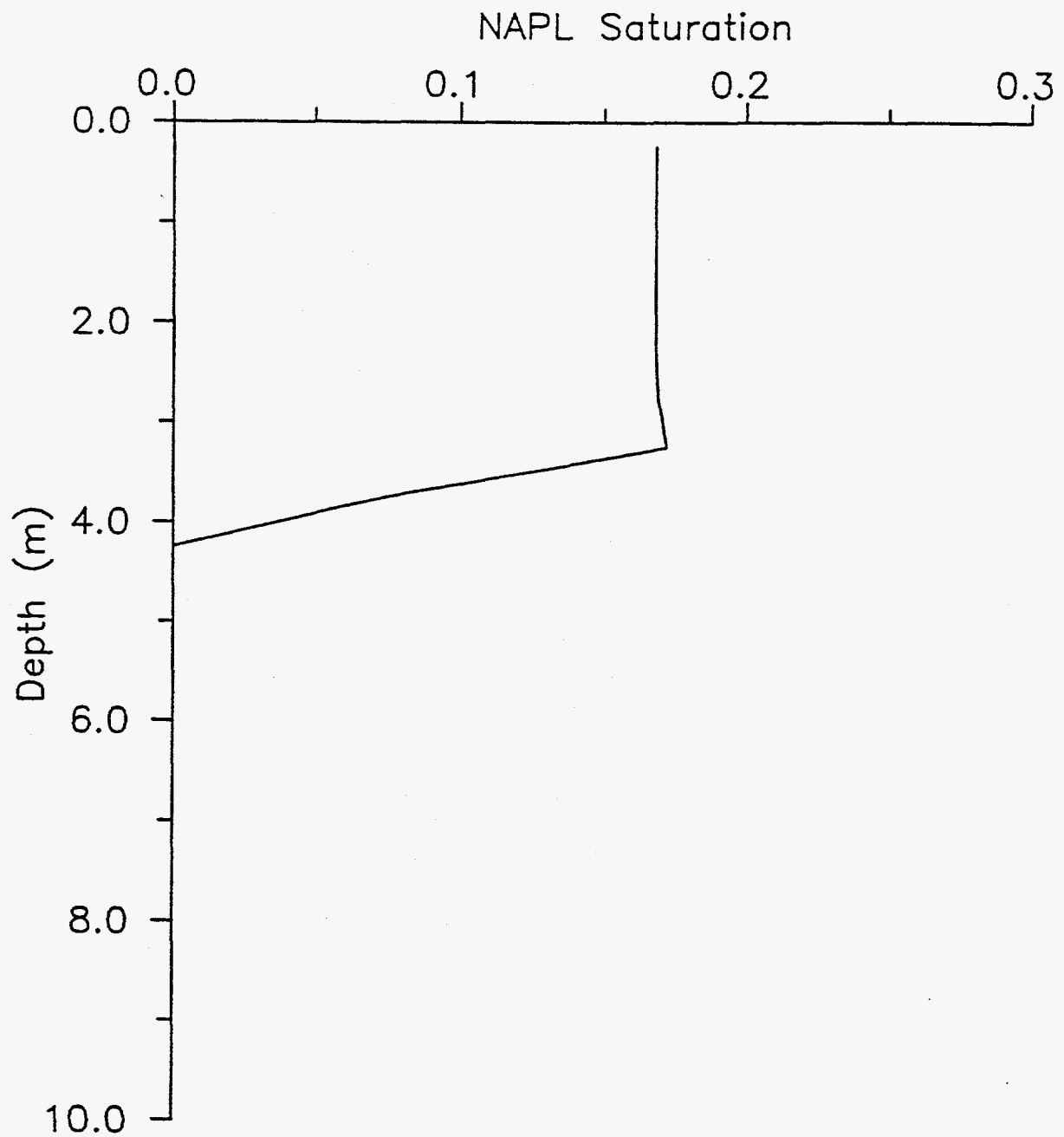


Figure 4.34. Steady-state profile of LNAPL saturations obtained for the one-dimensional multiphase transport problem.

single-component LNAPL was assumed to be slightly soluble in water and air. A schematic description of the transport problem is shown in Figure 4.35. The transport parameter values used are listed in Table 4.13. 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 4.36, 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 and vaporization of the immobile LNAPL mass. Shown in Figure 4.37 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 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.

4.5.2 Two-Dimensional Transport of Dissolved Mass of LNAPL Spill

This problem was selected to demonstrate an application of SAMFT2D to a two-dimensional multiphase transport problem. The situation of interest concerns transport of single-component LNAPL contaminant in an unconfined groundwater system subjected to a steady and

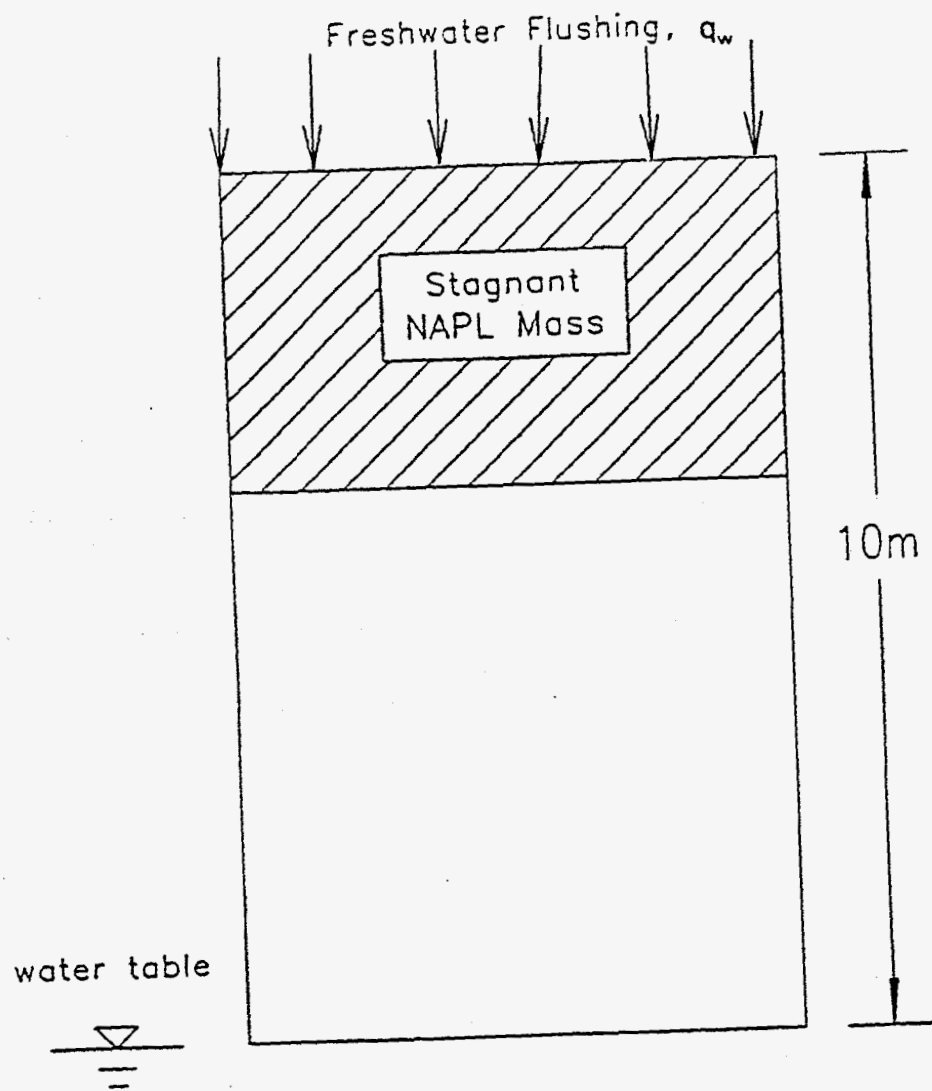


Figure 4.35. Schematic description of the one-dimensional multiphase transport problem.

Table 4.13. Parameter values used in the one-dimensional multiphase transport simulation.

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 limit, c_{ws}	0.01
Henry's constant, κ_a	0.25
Degradation coefficient, λ	0
Longitudinal dispersivity, α_L	1 m
Tortuosity, τ	0.58
Water diffusion coefficient, D_{mw}	8.64 x 10 ⁻⁵ m ² /d
Air diffusion coefficient, D_{ma}	0.864 m ² /d

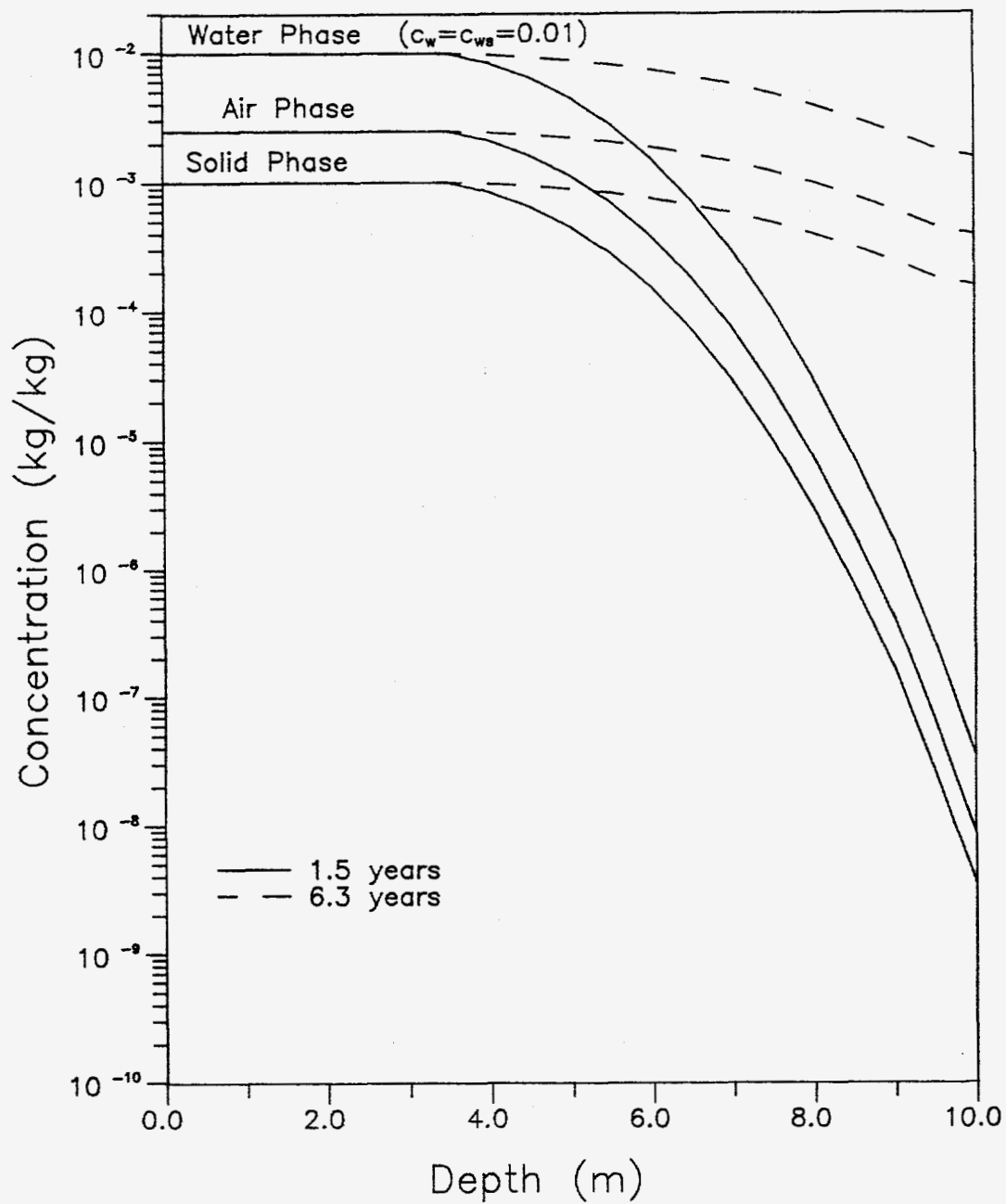


Figure 4.36. Concentration profiles for the 1-D multiphase transport problem.

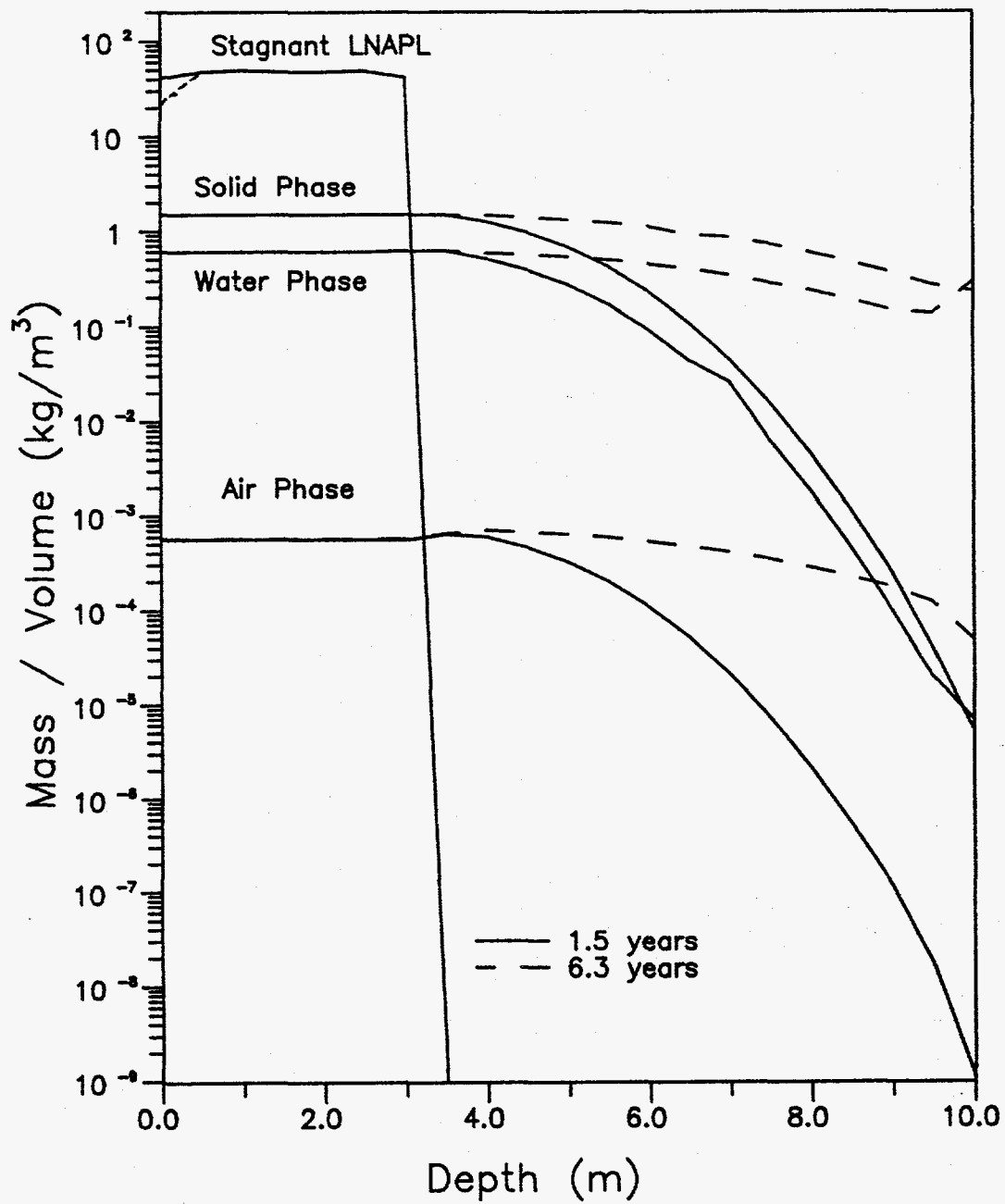


Figure 4.37. Distributions of contaminant mass for the 1-D multiphase transport problem.

uniform recharge. As depicted in Figure 4.38, an accidental spill of limited quantity of LNAPL on the ground surface provided a discontinuous LNAPL source. The LNAPL mass migrated into the unsaturated zone and was eventually captured by capillary forces. The immobile LNAPL zone shown in Figure 4.38 was delineated by conducting a three-phase flow simulation in a similar manner to that described in Section 4.5.1.

The flow domain and boundary conditions are depicted in Figure 4.38. The domain was discretized using a uniform grid consisting of 240 elements and 273 nodes ($\Delta x = 1.408$ m, and $\Delta y = 0.25$ m). The LNAPL leakage rate was assumed to be 2.466 kg/d and over a 30-day duration. All material parameter values and the initial condition of the flow problem were kept the same as those given in Section 4.4.5.

Following the flow simulation, the single-component transport simulation was performed with the stagnant LNAPL mass represented as "the precipitated mass." The transport parameter values are given in Table 4.14. The simulation was performed over a period of 15 years. Shown in Figure 4.39 are the model predictions of the shrinking LNAPL zone and aqueous-phase concentrations at three typical time values. The shrinkage of LNAPL zone is due to dissolution and advective-dispersive transport in the mobile water and air phases. The contaminant transport in the saturated zone is farther downstream from the source due to the horizontally dominated groundwater velocity.

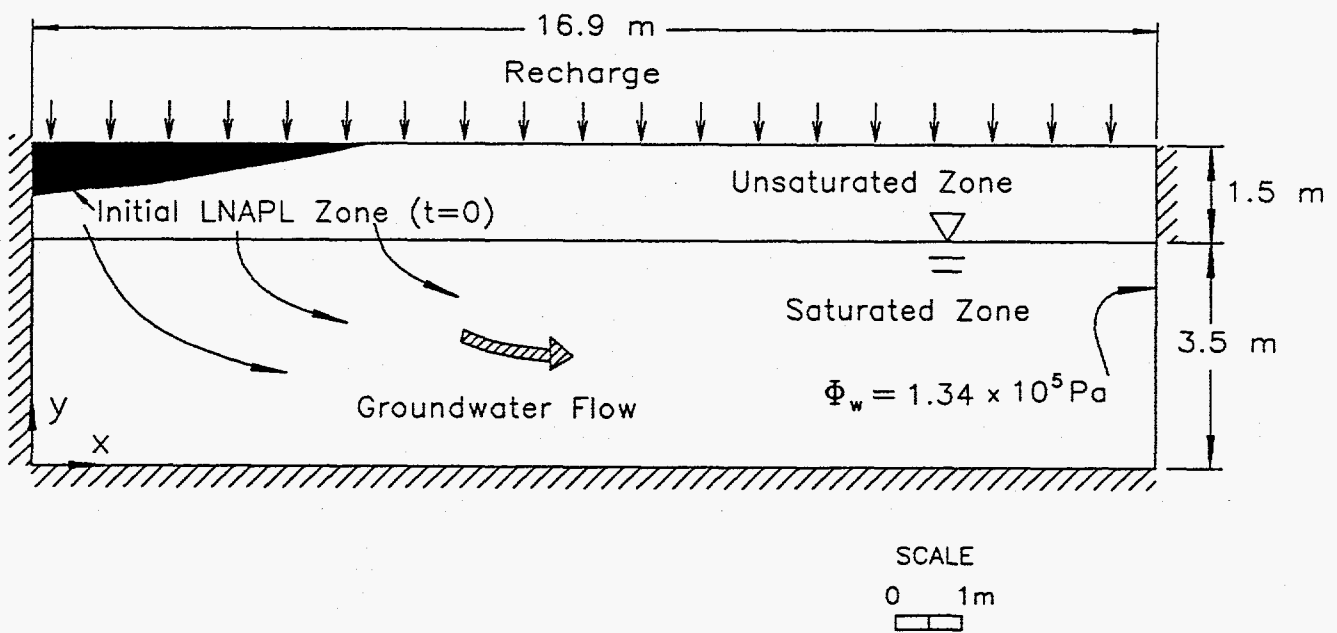
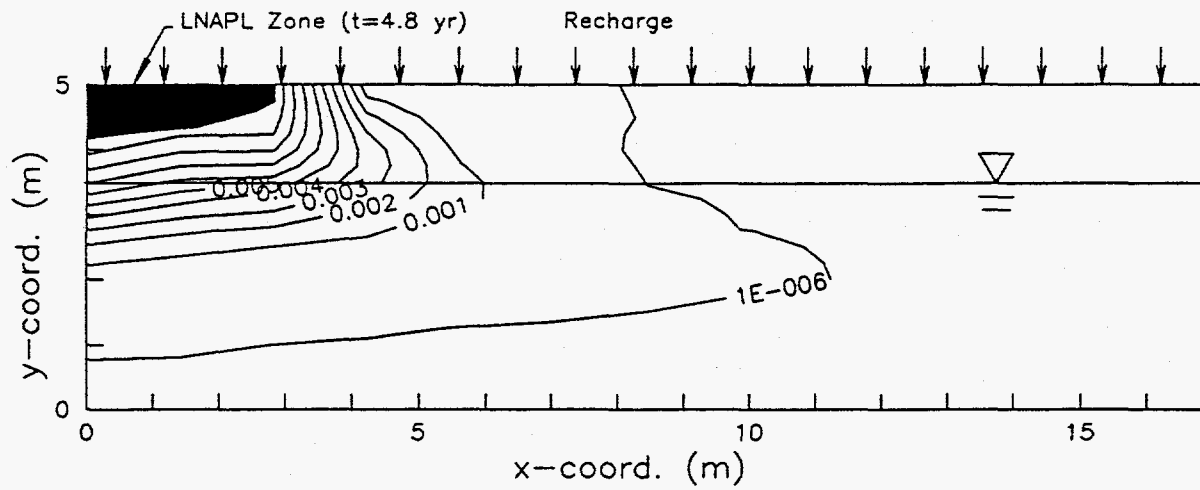


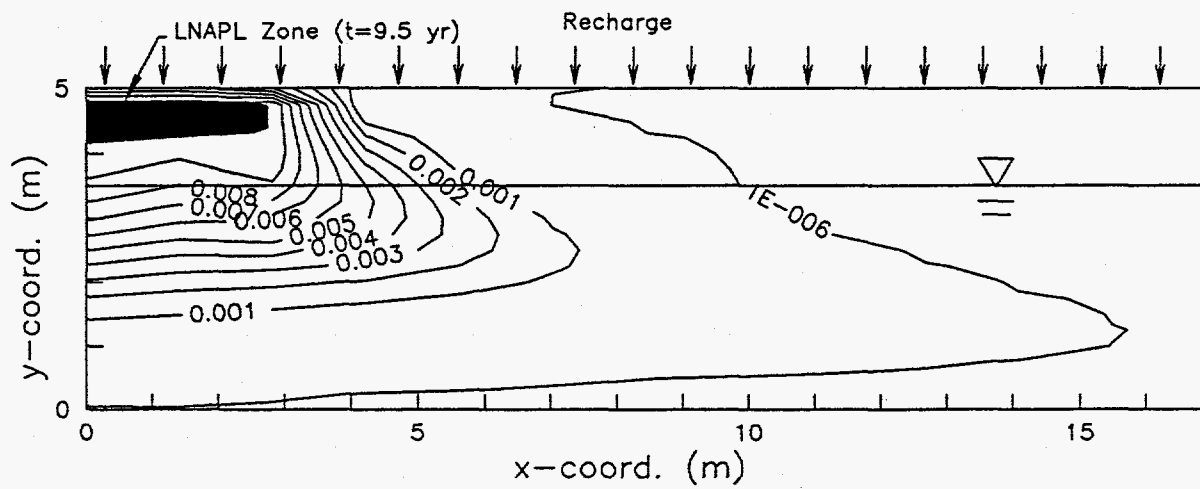
Figure 4.38. Schematic description of the two-dimensional multiphase transport problem.

Table 4.14 Parameter values used in the two-dimensional multiphase transport simulation.

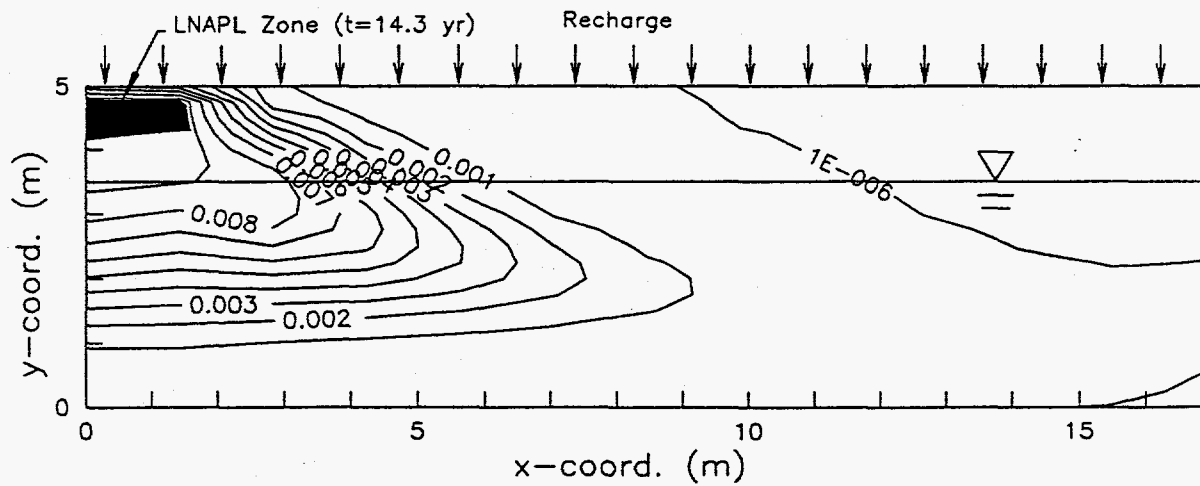
Parameter	Value
Effective porosity, ϕ	0.3
Water density, ρ_w	1000 kg/m ³
LNAPL density, ρ_n	950 kg/m ³
Air density, ρ_a	1.18 kg/m ³
Soil bulk density, ρ_B	1500 kg/m ³
Distribution coefficient, k_d	0.0001 m ³ /kg
Water-solubility limit, c_{ws}	0.01
Henry's constant, κ_a	0.25
Degradation coefficient, λ	0
Longitudinal dispersivity, α_L	0.5 m
Transverse dispersivity, α_T	0.005 m
Tortuosity, τ	0.58
Water diffusion coefficient, D_{mw}	8.64 x 10 ⁻⁵ m ² /d
Air diffusion coefficient, D_{ma}	0.864 m ² /d



(a)



(b)



(c)

Figure 4.39. Model predictions of the shrinking LNAPL zone and aqueous-phase concentrations at three typical time values, (a) $t = 4.8$ yr, (b) $t = 9.5$ yr., and (c) $t = 14.3$ yr.

5 PROBLEM DEFINITION AND SIMULATION PROCEDURE

5.1 TYPES OF PROBLEMS

The SAMFT2D code can be used in several types of investigations of fluid flow and contaminant transport in the subsurface. For demonstrative purposes, four typical examples are described. The first example concerns subsurface contamination due to disposal, leakage or accidental spillage of NAPL (NonAqueous Phase Liquid) chemicals. Shown in Figure 5.1 is a common scenario involving light NAPL with density less than that of water. For such a situation, the multiphase computational modules of SAMFT2D can be utilized. The multiphase flow module will predict the distribution of NAPL mass in the unsaturated and saturated zones of the unconfined system. The corresponding multiphase transport module will predict the rate of plume migration and concentration distributions of dissolved chemical components.

The second example (Figure 5.2) has application to the conceptual design and risk assessment for a low-level radioactive waste disposal site. It involves variably saturated flow around gravel and wick layers surrounding a low-level radioactive waste container placed in the unsaturated zone above a water table (Frind et al., 1977). For this study, SAMFT2D can be used to predict the flow pattern resulting from vertical recharge at the soil surface. The velocity field determined from flow simulations can be used as input to subsequent contaminant transport simulations. For the investigation or risk analysis of the potential for migration of radionuclides, SAMFT2D can be used to perform single-species transport simulations.

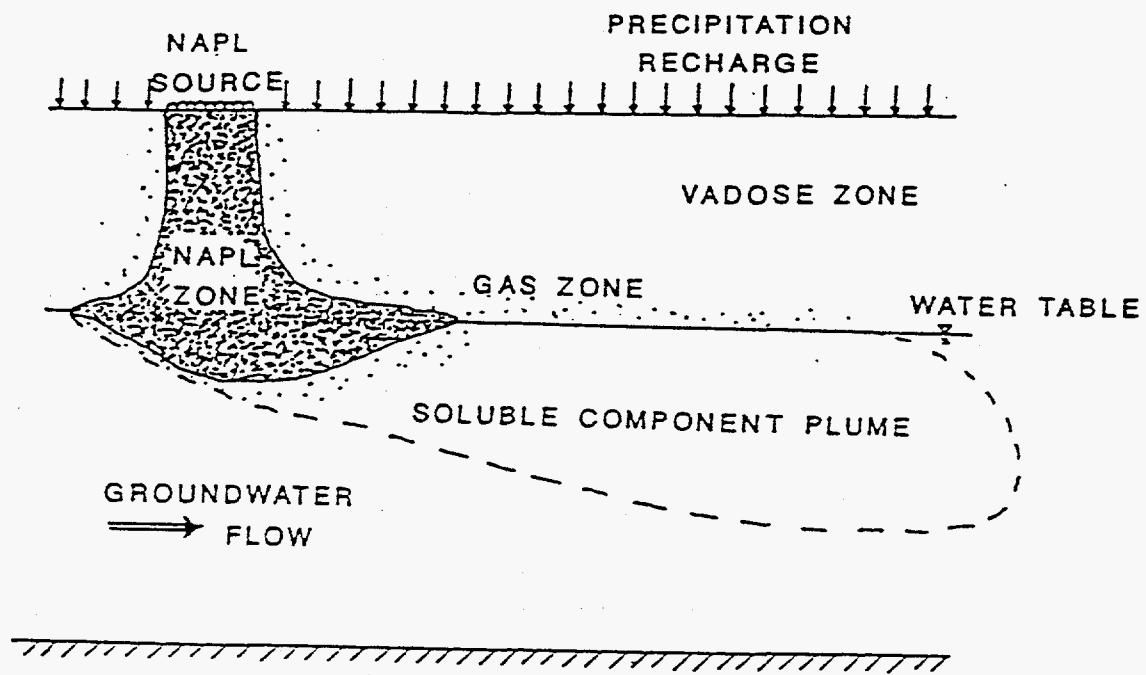


Figure 5.1. Schematic description of the distribution of nonaqueous phase liquid with density less than water and the soluble component plume.

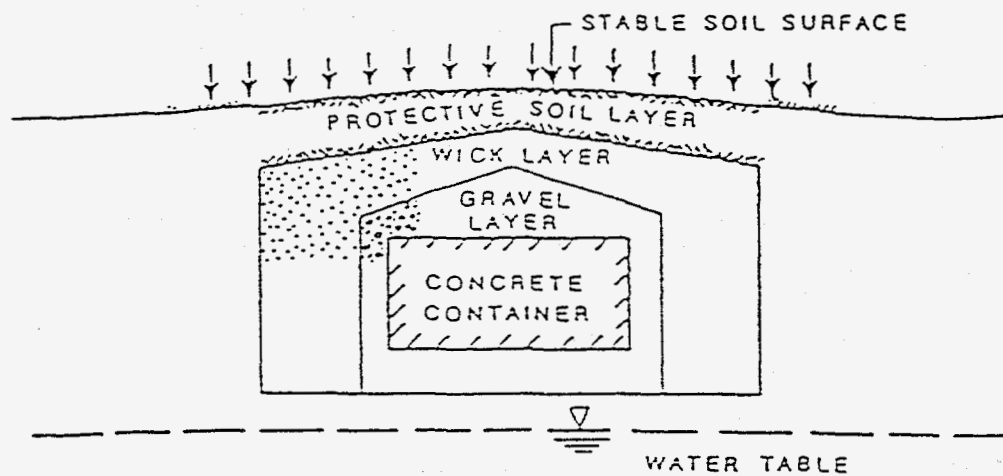


Figure 5.2. Basic geologic environment for a low-level waste container (Frind et al., 1977).

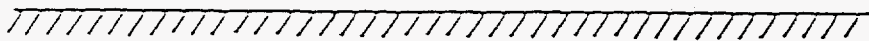
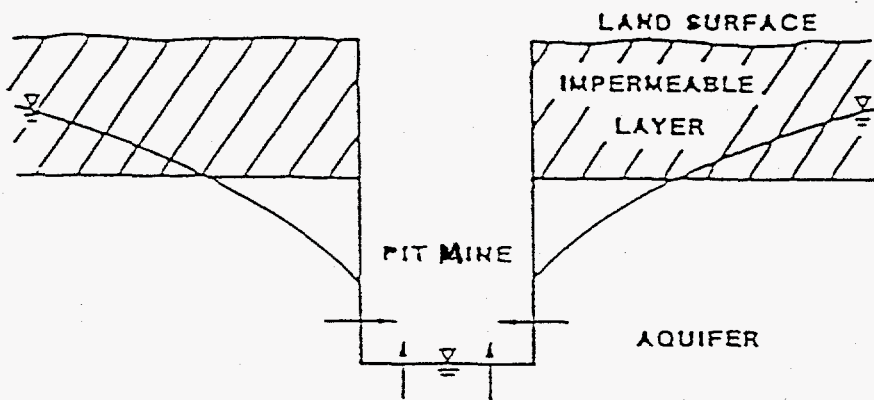
The third example (Figure 5.3) applies to drainage or mine dewatering problems involving analyses of seepage into a drain or mine pit. For this example, SAMFT2D can be used to perform saturated-unsaturated flow simulations taking into account groundwater recharge and seepage boundary conditions.

The fourth example applies to a landfill above an unconfined groundwater system intercepting a river (Figure 5.4). To evaluate the environmental impact of a land disposal unit (landfill or surface impoundment), it is essential to predict water flow and contaminant migration in both unsaturated and saturated zones between the landfill and the river. SAMFT2D can be used to perform both the flow and transport simulations.

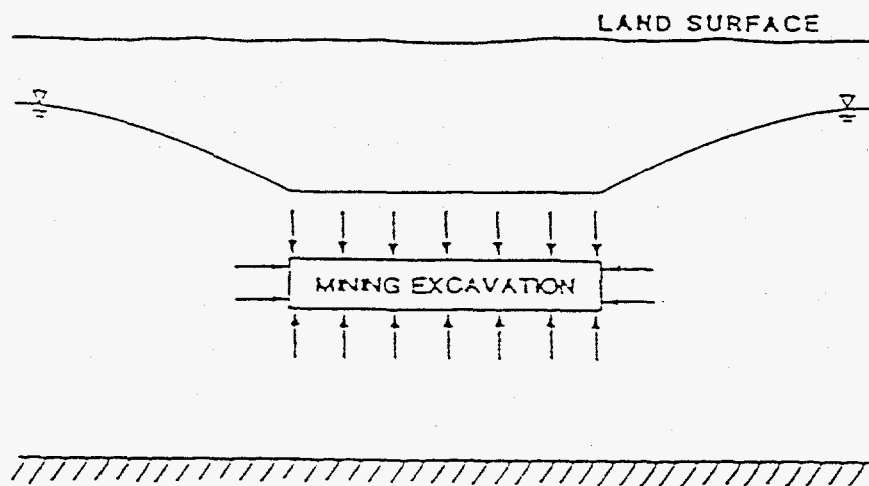
5.2 DATA REQUIREMENTS

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 of the porous medium needs to be supplied to the code either in a functional form or tabulation.

Data required for the simulation of solute transport includes longitudinal and transverse dispersivities of the porous media, solute properties (i.e., distribution and decay coefficients), information on groundwater recharge and withdrawal, as well as contaminant source characteristics (source location, geometry, concentration, and fluxes) Darcy velocity components and saturation of each active fluid phase, and initial and boundary conditions associated with the single-species transport equation.



(a)



(b)

Figure 5.3. Groundwater seepage due to mine dewatering or underground drainage operations.

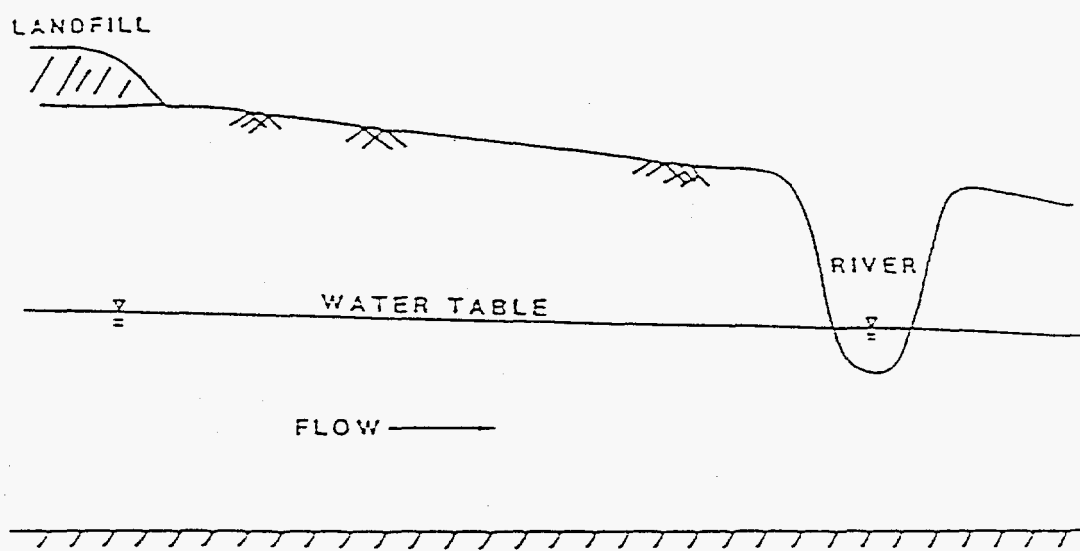


Figure 5.4. Groundwater contamination caused by a landfill.

5.3 SIMULATION PROCEDURE

The general procedure for using SAMFT2D 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 through 5.4. 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 a sketch of a given region showing the orientation of the coordinate axes and sequential numbers of the nodes and the elements (Figure 5.5).
- 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 SPECIFICATION OF MESH PARAMETERS

A rectangular mesh is used by SAMFT2D and the mesh is automatically generated by the code when the following mesh parameters are specified:

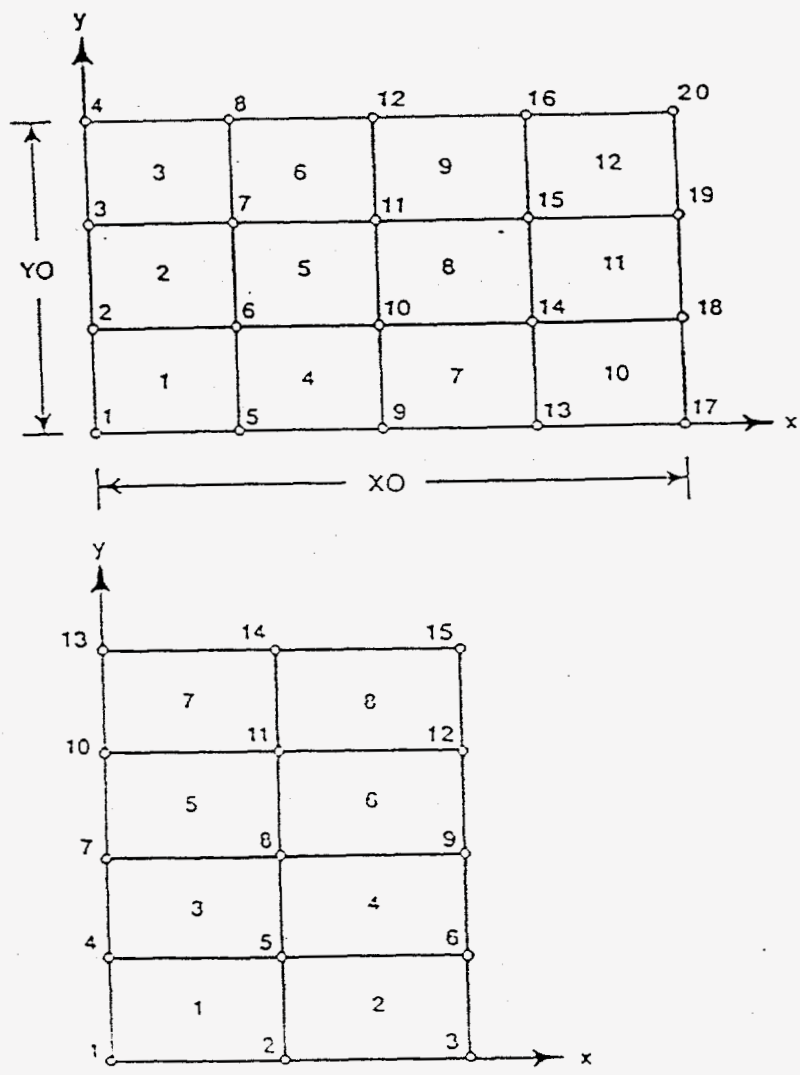


Figure 5.5. Typical rectangular meshes generated automatically by the SAMFT2D code using the option of IXYZRD = 0.

Record type 12 (see Chapter 8)

- NROWS: Number of grid lines parallel to x-axis.
- NCOLS: Number of grid lines parallel to y-axis.
- DXMAX: Maximum value of spatial increment allowed in x-direction.
- DYMAX: Maximum value of spatial increment allowed in y-direction.
- IXYZRD: Parameter for indicating if the grid line coordinates are to be input or generated by the code;
= 0 if coordinates are to be computed using generated values of spatial increments,
= 1 if coordinate input is needed,
= 2 if coordinates are to be computed using specified values of spatial increments.
- IHORGR: Parameter indicating if the grid is in a horizontal plane;
= 1 if yes,
= 0 if no.

Note how the nodes are sequentially numbered in Figure 5.5 to achieve a minimum matrix bandwidth. The parameter that specifies how the nodes are to be numbered is ISWAP in record group 3, cols. 66-70.

Although SAMFT2D requires the use of rectangular mesh, the code allows an irregular region to be treated in a convenient manner. To achieve this, the user needs to overlay the selected regular and the modeled region. Elements that are outside the interested region can then be blocked out by zeroing components of the property array IPROP that correspond to such elements.

5.5 INITIAL AND BOUNDARY CONDITION SPECIFICATIONS

To perform a transient (single-phase or multiphase) analysis or a steady-state (single-phase only) 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).

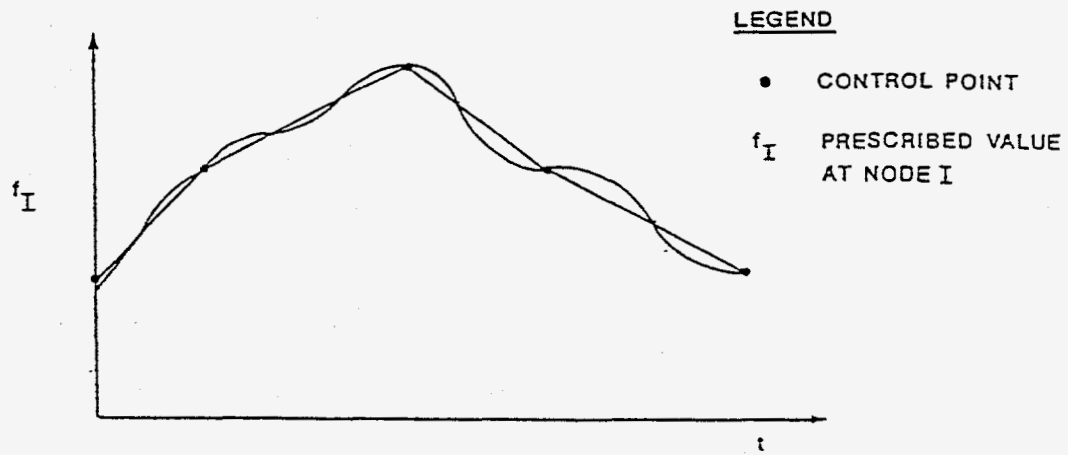
For a general case of nonuniform initial distribution, it is necessary to supply initial nodal values to the code. The number of nodes where initial values differ from the default value (NPIN) may be less than or equal to the total number of nodes (NP). The input initial values are used by the code to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

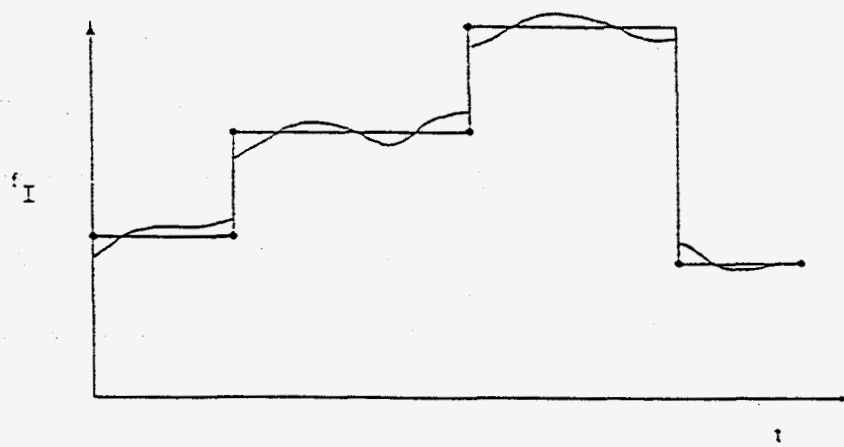
For a fluid flow analysis, the fluid flux at a node corresponds to the mass flow rate of the concerned fluid over the effective flow area covered by the node (assuming that the width normal to the x-y plane is one unit). The sign convention for flux adopted by the code is positive for influx and negative for efflux.

For a solute transport analysis, the solute flux at a node corresponds to the rate of solute mass entering the node over the effective flow area covered by the node (assuming that the width normal to the x-y plane is one unit).

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 5.6). 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.



(a)



(b)

Figure 5.6. Modeled approximations for continuous and discontinuous variations of prescribed function at node I.

6 CODE STRUCTURE

6.1 CODE ORGANIZATION AND MODULE DESCRIPTION

The SAMFT2D code is structured to accommodate two sets of computational modules designed to perform single-phase and multiphase analyses, respectively. The single-phase modules, which have been fully developed and incorporated into the current version of the code, 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: Water flow simulation only, solute transport simulation or dual simulation of flow and transport. A grid consisting of linear rectangular elements is generated and used by the code to represent the region of interest. The solutions of the matrix equations resulting from finite element discretizations of the flow and transport equations are performed using direct solvers designed especially for symmetric and asymmetric banded matrices. Nonlinear treatment of the variably saturated flow problem is performed using the Picard or Newton-Raphson scheme described in Chapter 3. An option of mass balance computation is available for both flow and transport analysis.

6.2 INTERNAL DATA STRUCTURE

Data necessary for the finite element analysis performed by the code is classified as follows:

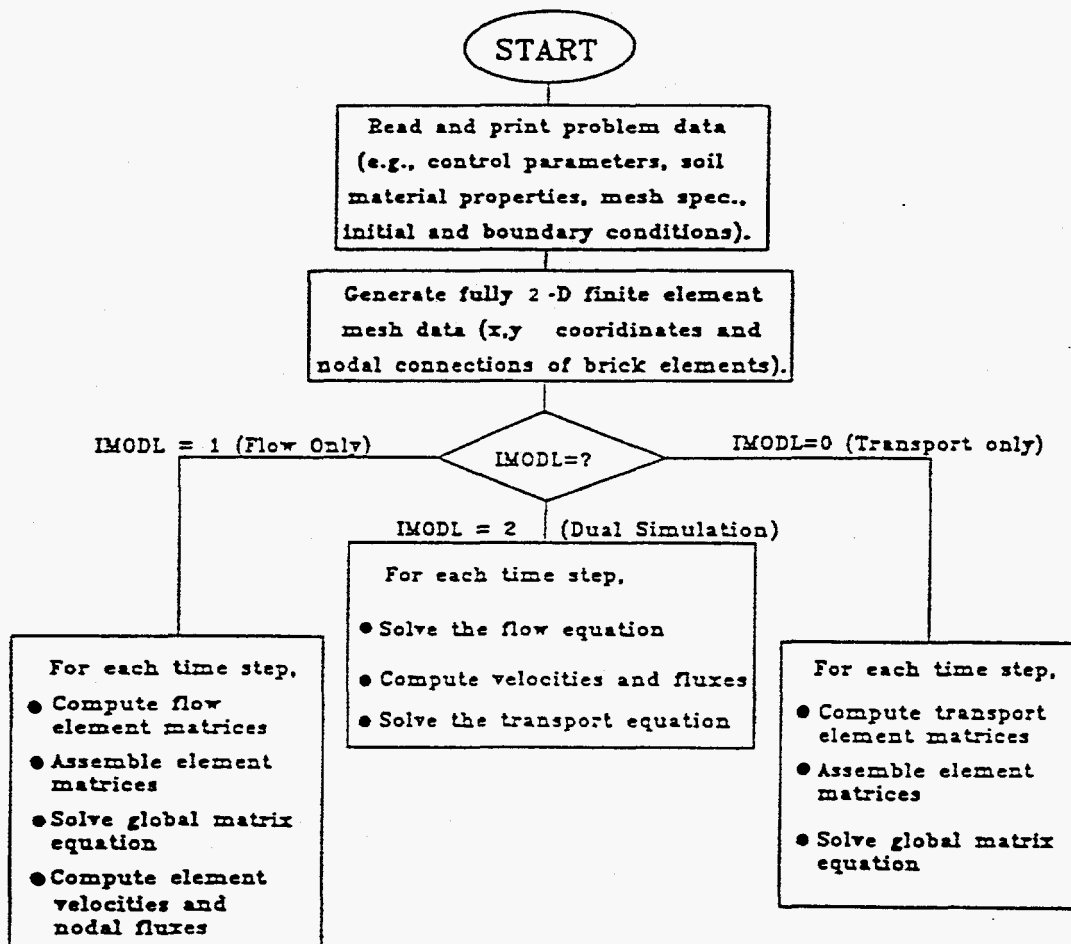


Figure 6.1. Flow chart for the SAMFT2D computational module.

(1) Material properties. The material properties pertaining to single or multiphase flow and transport analyses are read in and stored in three common blocks labeled MDATA, MADATB and MDATC, respectively.

(2) Mesh data and element material numbers. The mesh data generated by the code and the element material numbers are stored in a common block labeled MSHDAT.

(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 values of the dependent variables to be solved. 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.

(4) Initial condition data and computed nodal values of the dependent variables. These are stored in a common block labeled WAVE1.

(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 a common block labeled VSPDAT.

(7) Control parameters. Various control parameters of the problem and simulation are stored in six common blocks labeled CONTR1 through CONTR6.

(8) Global coefficient matrix. This matrix is generated and modified during simulation. It is stored in a common block labeled WDUM.

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. Note NDOFN denotes number equations per node. For flow problem $NDOFN = NMPHAS$ (the number of active phases). For transport problem, $NDOFN=1$.

Maximum total number of nodal points	= 2700/NDOFN
Maximum number of rectangular elements	= 2000
Maximum number of time steps	= 200
Maximum number of different sets of material properties	= 20
Maximum number of steady-state Dirichlet boundary conditions	= 1777
Maximum number of steady-state flux boundary conditions	= 1777
Maximum bandwidth of global coefficient matrix	= 75
Maximum number of time-dependent, Dirichlet boundary nodes	= 100
Maximum number of time-dependent, flux boundary nodes	= 100
Maximum number of nodes for which flux computation is required	= 1000
Maximum number of observation nodes	= 50

7 DATA FILES

7.1 MAIN INPUT AND OUTPUT FILES

There are two major input and output files used by the SAMFT2D 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. Two of these files contain binary (unformatted) records written on units 8 and 9, and the other two contain formatted records written on units 10 and 11. These files are described below.

1. File number 8. This is the backup output file containing nodal values of the dependent variables that were computed at the final time step of the current run. Information in this file can be used as the initial condition 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, written in the FORMAT (20A4)
- List of nodal values of the dependent variables at the final time level. These nodal values are written in the FORMAT (5E15.6).

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 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 binary 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
- List of storage capacity values at the nodes. This information is written only when the mass balance calculation option, IMBAL, is set equal to 1
- List of volumetric fluid fluxes at specified node. This information is written only when NBOU is greater than 0.

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 2. This directs the code to read velocity data from the file on unit 9
- Make sure that IMBAL and IOUFLT in record group 5 for fully 3-D option is set to the value used in the flow simulation. This is necessary to insure compatibility of FORMAT and avoid I/O format error.

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 (20A4)
- Nodal x and y coordinates and values of the dependent variables (4E15.6).

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 (20A4)
- (x, y) coordinates of the element centroids and components of Darcy velocity (5E15.6).

8 INPUT DATA PREPARATION

8.1 GENERAL CONSIDERATIONS

SAMFT2D 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 SAMFT2D for automatic generation of a substantial portion of input required for the finite element analysis of a single-phase or multiphase problem. These are summarized below.

- (1) Mesh generation option. A rectangular finite element grid is generated automatically by the code. The grid has a constant number of nodal rows and columns. Nodal spacings along the x and y axis may be uniform or variable. The x-axis is oriented in a horizontal direction. The y-axis may be oriented in a horizontal or the upward vertical direction depending on the problem configuration. The complete mesh data generated by the code consists of nodal coordinates and element nodal connections.
- (2) Default initial value option. This option may be invoked by setting an input control parameter NONU=0. When this is the case, all nodal values of the primary dependent variables will be set equal to the default initial values.
- (3) Time step generation option. Time steps to be used in the finite element analysis of a transient problem can also be generated

automatically. This option may be invoked by setting an input control parameter ITSGN=1 or 2.

- (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 SAMFT2D 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. Note that in SAMFT2D a unit width or length in the normal direction to the flow plane is used in the flux computation.
- (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 active fluid phases considered 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 DATA PREPARATION GUIDE

The main stream of input data required for a flow simulation or a transport simulation is to be supplied from a FORTRAN input file on unit 5. To facilitate data entry, the input data for each problem is divided into 22 groups and arranged as follows:

1. Problem control record
2. Problem title record
3. Simulation control record
4. General and time stepping control record
5. Input/output control record
6. Temporal discretization data
7. Default initial condition data
8. Element material numbers
- 9-I. Material properties for flow simulation
- 9-II. Additional Data for hysteretic flow simulation
10. Material properties for transport simulation
11. Mesh parameter specification
12. Grid line coordinates
13. Coordinate generation parameters
14. Boundary condition data
15. Transient Dirichlet boundary condition data
16. Transient flux boundary condition data
17. Initial condition data

3. Simulation control parameters (1515)

One record.

Col. 1-5	IMODL:	Parameter indicating the type of modeling required; = 0 for solute transport modeling, = 1 for variably saturated flow modeling, = 2 combined variably saturated 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 whose governing equations need to be solved. Note that $NMPHAS \leq NTPHAS$. For a single-phase flow problem, set $NMPHAS = 1$.
16-20	IMNUMR:	Parameter indicating if data concerning porous material number specification (group 8) is to be input; = 1 if yes, = 0 if no. Set $IMNUMR = 0$ if dealing with a rectangular flow domain with entirely homogeneous material properties.
21-25	NVAR:	Number of primary variables for which nodal values are to be computed; = 1 if $IMODL = 0$, = $NMPHAS$ if $IMODL = 1$, = $NMPHAS + 1$ if $IMODL = 2$.
26-30	ISSTA:	Parameter indicating a steady-state analysis of the problem is to be performed; = 1 if yes, = 0 if no. Set $ISSTA = 0$ if performing a multiphase simulation.

31-35	ITSGN:	<p>Parameter indicating if simulation time values are to be generated by the code;</p> <p>= 0 if no and simulation time values are to be supplied to the code,</p> <p>= 1 if yes and computational time step values are to be determined by the code during the flow simulation based on the rate of nonlinear convergence,</p> <p>= 2 if yes and time step values are to be supplied to the code.</p> <p>Note: the option of ITSGN = 1 is to be used for cases involving flow simulation (IMODL = 1) or combined flow/transport simulation (IMODL = 2).</p>
36-40	NTS:	<p>Number of time steps. Set NTS = 1 if a steady-state analysis is required.</p>
41-45	NP:	<p>Total number of nodal points in the finite element grid.</p>
46-50	NE:	<p>Total number of elements in the grid.</p>
51-55	NMAT:	<p>Number of different porous materials.</p>
56-60	KPROP:	<p>Parameter indicating the form of relative permeability and capillary pressure data;</p> <p>= 0 for functional form,</p> <p>= 1 for tabulated form.</p> <p>KPROP must be set to 0 when dealing with single-phase flow problem.</p>
61-65	NONU:	<p>Parameter indicating if the initial condition differs from the default initial condition data described in record group 7;</p> <p>= 0 if no,</p> <p>= 1 if yes and initial condition data are to be supplied to the code as part of this input file (see group 17),</p> <p>= 2 if yes and initial condition data are to be read from a file on unit 8.</p>

66-70 ISWAP: Parameter indicating the sequential numbering of the nodes in each gridding plane of the mesh;
= 1 if the nodes are sequentially numbered in the x-direction,
= 0 if the nodes are sequentially numbered in the y-direction.

71-75 IHYST: Parameter indicating if hysteresis is to be included in the single-phase, variably saturated transient 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.

4. Time stepping, iteration control and gravitational parameters (2I5,5E10.3, 2I5)

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 transport 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 = 5 and 20 for transient and steady-state simulations, respectively.

11-20 HTOL: Equivalent freshwater head tolerance to be used in the solution of nonlinear flow equations. Suggested value is $0.0 < HTOL \leq 0.01$ m.

21-30	STOL:	Saturation tolerance to be used in the solution of nonlinear flow equations. Suggested value is $0.0 < \text{STOL} \leq 0.005$.
31-40	CTOL:	Concentration tolerance to be used in the solution of multiphase transport equation.
41-50	GCONST:	Gravitational acceleration constant.
51-60	PATM:	Atmospheric pressure.
61-65	IRESOL:	Maximum number of refinements of time steps allowed if the solution of the variably saturated flow equation does not converge (recommended value is 3 or 4). Leave blank if transport simulation only is required (IMODL=0).
66-70	IPICRD:	Parameter indicating if Picard scheme is to be used in the nonlinear solution of single phase flow problem, = 1 if yes, = 0 if no. Set IPICRD=0 if dealing with a multiphase flow problem.

5. Input and output control parameters (14I5)

One record.

Col. 1-5	NVREAD:	Parameter specifying if element velocity 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:	Parameter indicating if boundary node data (see group 20) are to be input:

= 1 if yes,
= 0 if no.

IOUTLT is automatically set by the code to 1 if IMBAL = 1 (group 5, col. 46-50).

- 11-15 NPIN: Number of nodes for which initial 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 output requirement;
 = 0 if complete mesh data printout is required,
 = 1 if element connection data printout is not needed,
 = 2 if the whole mesh data printout is not needed,
 = 3 if mesh and initial condition data printouts are not needed.
- 21-25 NVWRIT: Parameter specifying if the computed values of element velocities 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 selected time steps as specified in record group 22b.
- Note: set NVWRIT = 0 if 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 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 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 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 group 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: Matrix computation print check parameter (used for debugging purposes);
 = 0 if print-check is not needed,
 = 1 if print check is needed.
- 61-65 IPWOUT: Parameter indicating the output requirements for single-phase flow analysis;
 = 0 if pressure-head values are to be printed,
 = 1 if pressure values at the nodes are to be printed.

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

*** Omit unless ITSGN = 2 (group 3, col. 31-35).

Number of records = as many as needed.

Each record contains the following information:

Col. 1-10	TMST:	Starting time value of simulation.
11-20	TMEND:	Final time value of the simulation.
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

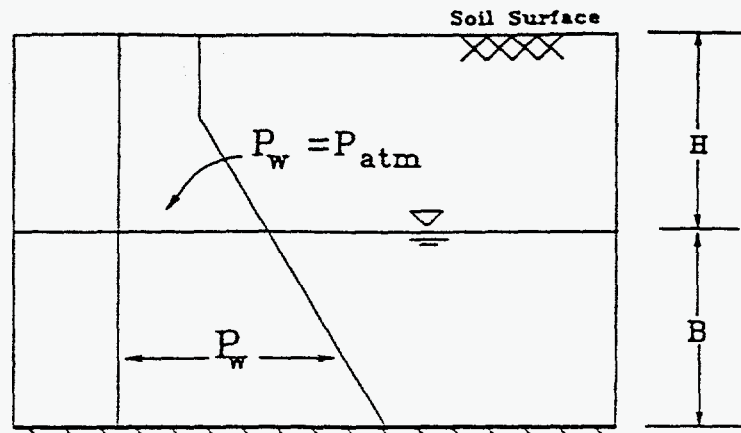
*** Omit if IMODL = 0 (group 3, col. 1-5).

The code provides four options for the specification of default initial condition for the simulation of fluid flow problem. The first three options are 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.

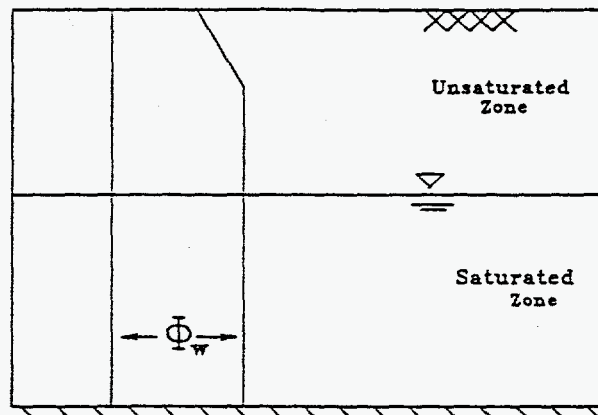
(i) First record (2I5,3E10.3)

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

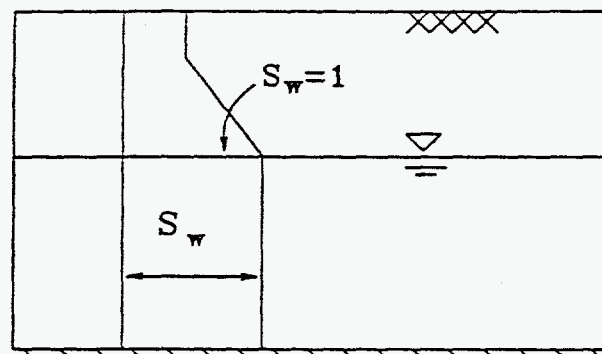
Col. 1-5	IDFVAR:	Initial condition identifier; = 1 if vertical profile of the initial pressure (p_w) of the first fluid phase (wetting phase) is to be specified (see Table 8.1 for the convention used in numbering fluid phases);
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(a) Prescribed initial 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.

- = 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; (This option is not to be used for the single phase flow problem.)
 - = 4 if dealing with horizontal flow problem for which initial distribution of water pressure is specified.
- Note that for single phase flow problem (NMPHAS = 1), IDFVAR should be set = 1, 2 or 4.

- 6-10 NCPONT: Number of control points required to specify the distribution of the initial function corresponding to the specified value of IDFVAR. Minimum value of NCPONT = 2.
- 11-20 HIDFAL(1): Default value of initial saturation of the second active fluid phase.
- 21-30 HIDFAL(2): Default value initial pressure of the third active fluid phase.
- 31-40 HIDFAL(3): Depth from the top of the model grid to the water table. Leave blank if the grid is horizontal.

(ii) Remaining records (2I5,2E10.3)

Number of records = NCPONT.

- Col. 1-5 N: Control point number (see Figure 8.2).
- 6-10 ISOIL(N): Soil material type identification number.
- 11-20 ZP(N): Value of coordinate along which the distribution of the initial function is specified (vertical y-coordinate if

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	--	--

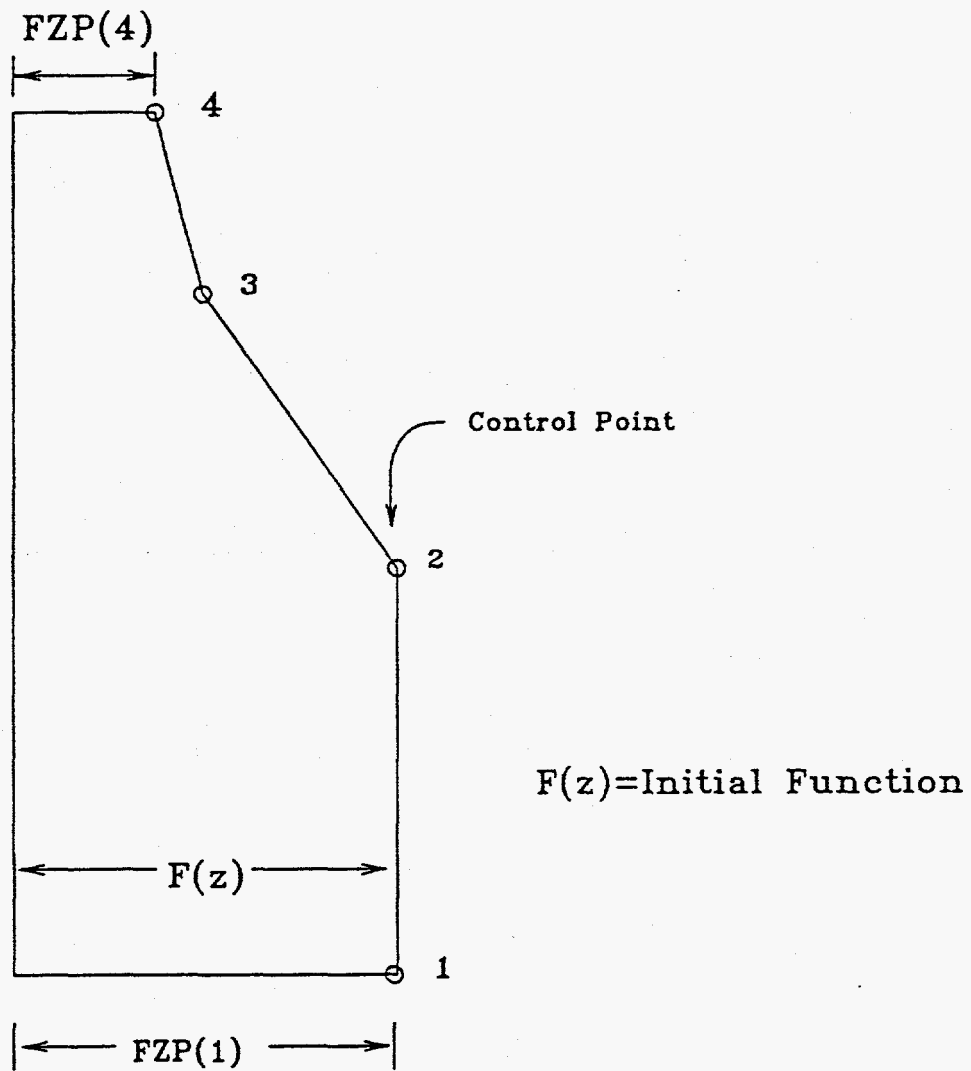


Figure 8.2. Representation of vertical profile of an initial function.

IDFVAR \leq 3 or horizontal x-coordinate 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, NCPONT) must be numbered sequentially starting from the minimum to maximum coordinate values of the flow domain.

(b) 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 dissolved concentration of the species component.

8. Material number specification

*** Omit this group if IMNUMR = 0 (group 3, col. 16-20).

Follow the instruction in parts (a) and (b) for single-phase and multiphase simulations, respectively.

(a) Single-Phase Simulation (5I5)

For single-phase flow and/or transport simulation, input the following data:

Number of records = as many as needed. Each record contains:

Col. 1-5	IMATNO:	Soil material number to be assigned to elements whose element numbers are in the range specified in this record.
6-10	IELST:	Starting element number.
11-15	IELEND:	Ending element number.
16-20	IELINC:	Element number increment for IMATNO assignment.

21-25 IPAUSE: Parameter indicating if this is the last record of group 8;
 = 1 if yes,
 = 0 if no.

Note: Elements that are outside the flow domain or in the impermeable zone need not be specified. The code automatically assigns their IMATNO as zero.

(b) Multiphase Simulation (5I5)

For multiphase flow and/or transport simulation, input the following data:

Number of records = as many as needed. Each record contains:

Col. 1-5	IMATNO:	Soil material number to be assigned to nodes whose node numbers are in the range specified in this record,
6-10	INDST:	Starting node number.
11-15	INDEND:	Ending node number.
16-20	INDINC:	Node-number increment for IMATNO assignment.
21-25	IPAUSE:	Parameter indicating if this if the last record of group 8; = 1 if yes, = 0 if no.

Note: Nodes that are outside the flow domain or in the impermeable zone need not be specified. The code automatically assigns their IMATNO as zero.

9-I. Material properties for flow simulation

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

(a) Soil properties (8E10.3)

Number of records = NMAT (group 3, col. 51-55)

Col. 1-10	PROP(I,1):	Intrinsic permeability component k_{xx} of material I.
11-20	PROP(I,2):	Intrinsic permeability component k_{yy} of material I.
21-30	PROP(I,3):	Intrinsic permeability component k_{xy} of material I.
31-40	PROP(I,4):	Volume compressibility of material I.
41-50	PROP(I,5):	Effective porosity of material I at reference pressure.
51-60	PROP(I,6):	Air-entry pressure head for the water-air (w-a) system, $\psi_a = 0$.
61-70	SNIRWN(I):	Irreducible NAPL saturation for the water-NAPL (w-n) fluid system.
71-80	SNSTR(I):	Threshold (critical) NAPL saturation beyond which air-water interface ceases to exist. Default value of SNSTR(I) is equal to that of SNIRWN(I).

Note: For an isotropic soil material, set $k_{xx} = k_{yy}$ and $k_{xy} = 0$. For single phase flow simulation, leave col. 51-70 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 page 2-18).

(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: $\bar{S}_w = [1 + (\alpha \psi - \psi_a ^\beta)]^{-\gamma}$ 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 $\gamma = 1-1/\beta$.
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. 71-75), 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 AKSTAR(I): Relative permeability of NAPL at the residual saturation of water in the water-NAPL (w-n) fluid system.

31-40 PCNWS1(I): Capillary pressure between fluid phases n and w at $S_w = 1$.

Note: Omit col. 21-40 if the total number of fluid phases (NTPHAS) is less than 3.

(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. 71-75).

(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.
	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 parameter (6E10.3)

Number of records = NMAT (group 3, col. 51-55)

Col. 1-10	PROPJ(I,1):	Longitudinal dispersivity, α_L , of soil material I.
11-20	PROPJ(I,2):	Transverse dispersivity, α_T , of soil material I.
21-30	PROPJ(I,3):	Tortuosity factor, τ , of material I.
31-40	PROPJ(I,4):	Exponent n of the equation: $D_l^* = (\phi \tau S_l^n)$ D_{ml} 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 $\tau = \phi^{1/3}$.
41-50	PROPJ(I,5):	Effective porosity, ϕ , of soil material I.
51-60	PROPJ(I,6):	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 fluid phase I. See Table 8.1 for fluid phase numbering convention
11-20	I=1,	
etc.	NTPHAS	

(c) Soil-solute transport parameters (5E10.3)

Number of records = NMAT (group 3, col. 51-55).

Col. 1-10	RPROP(I,1):	Solute decay coefficient, λ , of soil 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.
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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) = 0.

(d) Fluid Densities (3E10.3)

*** Omit if NMPHAS = 1 (group 3, col. 11-15)

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. Mesh parameter specification (2I5,2F10.3,2I5)

One record.

Col. 1-5	NROWS:	Number of grid lines parallel to the x-direction. NROWS must not be less than 2.
6-10	NCOLS:	Number of grid line parallel to the y-direction. NCOLS must not be less than 2.
11-20	DXMAX:	Maximum value of spatial increment allowed in the x-direction.
21-30	DYMAX:	Maximum value of spatial increment allowed in the y-direction.
31-35	IXYZRD:	Parameter indicating if x, and y coordinates of the grid lines are to be input or generated by the code; = 0 if coordinates are to be computed using generated values of spatial increments, = 1 if coordinate input is needed, = 2 if coordinates are to be computed using specified values of spatial increments.
36-40	IHORGR:	Parameter indicating if the grid is in a horizontal plane and gravity effect is to be neglected; = 0 if no (i.e., vertical cross-section), = 1 yes.

12. Grid line coordinates

*** Omit if IXYZRD = 0 or 2 (group 11, col. 31-35).

(a) Grid line x-coordinates (8F10.3)

Number of records = NCOLS/8+0 or 1 (group 11, col. 6-10).

Col. 1-10	XW(J) :	x-coordinates of grid lines 1 through
11-20	J=1,	NCOLS.
etc.	NCOLS	

(b) Grid line y-coordinates (8F10.3)

Number of records = NROWS/8 = 0 or 1 (group 11, col. 1-5).

Col. 1-10	YW(I) :	y-coordinates of grid lines 1 through
11-20	I=1,	NROWS.
etc.	NROWS	

13. Coordinate generation parameters

*** Omit if IXYZRD = 1 (group 11, col. 31-35).

(a) Coordinate parameters (8F10.3)

One record.

Col. 1-10	DX:	Nodal spacing in the x-direction of the first grid block.
11-20	DY:	Nodal spacing in the y-direction of the first grid block.
21-30	XO:	Maximum value of x-coordinate.
31-40	YO:	Maximum value of y-coordinate.
41-50	SCFX:	Mesh grading factor in the x-direction.
51-60	SCFY:	Mesh grading factor in the y-direction.
61-70	XSTART:	Minimum value of x-coordinate.
71-80	YSTART:	Minimum value of y-coordinate.

(b) Spatial increment data (F10.2,3I5)

*** Omit unless IXYZRD = 2 (group 11, col. 31-35).

Number of records = as many as needed.

First subset

Each record contains the following information:

Col. 1-10	DELTA X:	Spatial increment in the x-direction.
11-15	ISTC:	Starting element column number.
16-20	IENDC:	Ending element column number.
21-25	IPAUSE:	Parameter indicating if this is the last record in the subset; = 1 if yes; = 2 if no.

Second subset

Each record contains the following information:

Col. 1-10	DELTA Y:	Spatial increment in the y-direction.
11-15	ISTR:	Starting element row number.
16-20	IENDR:	Ending element row number.
21-25	IPAUSE:	Parameter indicating if this is the last record in the subset; = 1 if yes; = 0 if no.

- Note: (1) The last values of IENDC and IENDR must be equal to NCOLS-1 and NROWS-1 respectively.
(2) The sum of DELTAX*(IENDC-ISTC + 1) must be equal to (XO-XSTART).
(3) The sum of DELTAY*(IENDR-ISTR + 1) must be equal to (YO-YSTART).

14. Boundary condition data

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.

(a) Boundary condition control record (4I5)

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.

(b) Steady-state Dirichlet boundary condition data (2I5,E10.3,I5)

*** Omit if NBTO = 0 (group 14a, 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 pressure is prescribed (see Table 8.1). 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.
21-25	ISPBC(I):	Multiphase flow boundary condition identifier, (leave blank if irrelevant),

Table 8.2. Dependent-variable numbering convention used by the code, p_ℓ and q_ℓ denote pressure and flux of fluid phase ℓ , respectively, and q_c denotes solute mass flux.

Problem Type Description	Governing equation number and corresponding pair of dependent variable and associate material flux			
	1(w) or 1(c)	2(n) 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) system	(p_w, q_w)	(p_n, q_n)	-	-
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)	(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 , and
(c) = governing transport equation for solute component.

- = -1 if the node is to be treated outflow node for the specified fluid phase,
- = 1 if the node is to be treated as an inflow node,
- = 0 if the fluid is allowed to enter or leave the node.

(c) Steady-state flux boundary condition data (2I5,2E10.3)

*** Omit if NDFLUX = 0 (group 14a, 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 equation, MDEGF(I) corresponds to the identification number of fluid phase for which the flux is prescribed. 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 equation, FLUXVO(I) denotes fluid flux at the specified node. This flux corresponds to the flux of the specified fluid phase. For the transport equation, FLUXVO(I) corresponds to the solute mass flux injected 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 withdrawal well nodes and efflux boundary nodes. Hence such nodes can be excluded from group 14c.

(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 air phase.

15. Transient Dirichlet boundary condition data

*** Omit if NBHVAR = 0 (group 14a, col. 11-15).

Number of record sets = NBHVAR.

Each set contains the following records:

(a) Control record (5I5)

One record.

Col. 1-5	NDHVAR(I):	Node number concerned with a time-dependent Dirichlet boundary condition of a particular governing flow or transport equation.
6-10	MDEGBT(I):	For the fluid flow problem, MDEGBT(I) corresponds to the identification number of the fluid phase for which the pressure is prescribed. 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.

21-25 ITPBC(I): Multiphase flow boundary conditions identifier, (leave blank if irrelevant),
 = -1 if the node is to be treated outflow node for the specified fluid phase,
 = 1 if the node is to be treated as an inflow node,
 = 0 if the fluid is allowed to enter or leave the node.

(b) Time value records (8E10.3)

Number of records = $NTSNDH(I)/8 + 0$ or 1 (group 15a, col. 11-15).

Col. 1-10 11-20 etc.	TMHV(I,J): J=1, NTSNDH(I)	Sequential time values corresponding to the control points on the time graph depicting temporal variation of the prescribed dependent variable (fluid phase pressure or solute concentration).
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(c) Functional value records (8E10.3)

Number of records = $NTSNDH(I)/8 + 0$ or 1 (group 15a, col. 11-15).

Col. 1-10 11-20 etc.	HVTM(K,J): J=1, NTSNDH(I)	Prescribed values of the concerned variable (fluid phase pressure or solute concentration at the corresponding time values, TMHV(I,J)).
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16. Transient flux boundary condition data

*** Omit if NBFVAR = 0 (group 14a, 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. 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 records (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 nodal fluid flux of the specified fluid phase. For the transport equation, FVTM(I,J) corresponds to the solute mass flux injected at the node.
11-20	J=1,	
etc.	NTSNDF(I)	

(d) Fluid flux value records (8E10.3)

*** Omit if performing flow simulation only, IMODL = 1 (group 3, col. 1-5). Also omit if performing combined flow-transport simulation

(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 11-20 etc.	QVTM(I,J): J=1, TNSNDF(I)	Fluid flux values corresponding to TMHF(I,J). For a single phase simulation, this flux corresponds to volumetric water flux, Q_{wI} . For multiphase simulation, the flux corresponds to the total partitioned fluid flux, Q_{TI} , defined at the end of group 14.
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17. Initial condition data

*** Omit if NONU = 0 or 2 (group 3, col. 61-65). 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 (I5,4E15.6)

To be used only when NPIN (group 5, col. 11-15) is less than NP (group 3, col. 41-45).

(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 6-15 16-25 etc.	N: HINT(N,J): J=1,NVAR CMP(N):	Node number. Initial value of primary dependent variable number 1 through NVAR (group 3, col. 21-25). Table 8.3 provides the ordering of the primary variables for various simulations. Initial mass of the modeled species component considered to be in the precipitated phase per unit volume of porous medium at node N.
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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_w	S_n	S_w	(c)
Two-phase (w,n) flow in (w,n,a) fluid system	P_w	S_n (NAPL) saturation	(c)	
Two-phase (w,n) flow in (w,n) fluid system	P_w	S_w (water saturation)	(c)	
Single-phase water flow in (w,a) fluid system	P_w	(c)		
Single-component solute transport	c			

Note that for a combined flow/transport simulation, the concentration variable (c) is the additional variable following the flow variables.

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 (5E15.6)

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.

For record sets 1 through NVAR,

Number of records in each set = NP/5 + 0 or 1. Record set J contains:

Col. 1-10 11-20 etc.	HINT(I,J): I=1,NP	Initial values of primary dependent variable J at nodes 1 through NP. (See Table 8.3 for the ordering of primary variables).
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For multiphase transport simulation, the next record set contains:

Col. 1-10 11-20 etc.	CMP(I): I=1,NP	Initial values of precipitate mass of the contaminant at nodes 1 through NP.
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18. Transport simulation control data (I5,2F10.3)

*** 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 in x-direction. Leave blank if upstream weighting is not required.
16-25	YFAC:	Default value of transport upstream weighting factor in y-direction. Leave

blank if upstream weighting is not required.

19. Default velocity and phase saturation data (I5,3E10.3)

*** 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 Darcy velocity component of fluid IPHAS in the x-direction.
26-35	VYDFPH(IPHAS):	Default value of Darcy velocity component of fluid IPHAS in the y-direction.

20. Boundary nodal data

*** This record type is to be omitted if IOUTLT (group 5, col. 6-10) and IMBAL (group 5, col. 46-50) = 0 (i.e. flux and mass balance calculation is not required).

(a) Control record (I5)

One record.

Col. 1-5	NBOUT:	Number of nodes where integrated nodal flux values are to be computed.
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(b) Nodal numbers for flux computation (16I5)

*** Omit if NBOUT = 0.

Number of records = NBOUT/16 + 0 or 1.

Col. 1-5 6-10 etc.	NDOUT(I): I=1, NBOUT	Node numbers of the nodes for which integrated nodal flux values are to be computed.
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21. Observation node data

*** Omit if IOBSND = 0 (group 5, col. 41-45).

(a) Control record (I5)

One record.

Col.	1-5	NNOBS:	Number of nodes for which time history of computed values of dependent variable(s) is to be recorded.
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(b) Observation node numbers (16I5)

Number of records = $NNOBS/16 + 0$ or 1.

Col.	1-5	NDOBS(I):	Node numbers of observation nodes.
	6-10	I=1,	
	etc.	NNOBS	

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 (2E10.3,215)

*** Omit unless NVWRIT = 1 (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.
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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 22; = 1 if yes, = 0 if no.

9 OUTPUT

9.1 GENERAL CONSIDERATIONS

Line printer output from SAMFT2D 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 or user supplied mesh data
- Listing of boundary condition data
- Listing of initial condition data
- Listing of user-supplied steady-state values of element Darcy velocities and phase saturation
- Listing of user-supplied data pertaining to the nonzero flux nodes and flux values
- Listing of element numbers and centroidal coordinates
- Listing of the input data supplied from a backup file on unit 9 for each specified 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 computed values of the dependent variables. This listing is given for every n-th time step, where n is the value of NSTEP
- Listing of element numbers and saturation values. This listing is given for every n-th time step, where n is the value of NVAR
- Listing of element numbers and the x and y components of Darcy velocity for each active fluid phase. This listing is given for every n-th time step, where n is the value of NVPR.

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. Printed Output Control Parameters.

CONTROL PARAMETER	VALUE	MEANING
IPRD	3	Suppress the printout of the entire mesh data as well as the initial condition.
IPRD	2	Suppress the printout of the entire mesh data.
IPRD	1	Suppress the printout of element connectivities.
NSTEP	n	For each n-th time step, print computed values of head or concentration (as the case may be). 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 element liquid saturations and 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 on unit 5, described in Section 8.3.	

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 files and simulation output for five sample problems are provided. These are the one- and two-dimensional, single-phase and multiphase flow and transport problems.

The first problem (Section 10.2) was used to show the code's capability and options for simulating single-phase unsaturated flow including effects of hysteresis on capillary pressure. These options are: (1) automatic generation of mesh data and time steps, (2) default initial saturation values, (3) entry of hysteretic functional moisture retention 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 used to show the code's capability and options for simulating two-phase non-capillary (Buckley-Leverett type) flow of water and an immiscible liquid in a porous medium. These options are: (1) automatic generation of mesh data and time steps, (2) default initial condition for two-phase simulation, (3) entry of tabulated data for relative permeabilities, (4) specification of steady-state pressure and flux boundary conditions, (5) computation and printout of Darcy velocity components and saturation for each fluid phase, (6) mass balance computation, and (7) printout control options.

The third problem (Section 10.4) was used to show the code's capability and options for simulating vertical infiltration and transport of NAPL (Non-Aqueous Phase Liquid) contaminant in a three-phase (water, NAPL and air) fluid system. The exercised options are: (1) automatic generation of mesh data and time steps, (2) default initial conditions for simulation of two-phase flow in the three-phase fluid system, (3) entry of tabulated data for capillary pressures and relative permeabilities, (4) specification of steady-state pressure and flux boundary conditions, (5) computation of Darcy velocity components and saturations, (6) mass balance computation, and (7) printout control options.

The fourth problem (Section 10.5) was used to show the code's capability and options for simulating three-phase flow of water, NAPL and air in a porous medium. The exercised options are: (1) automatic generation of mesh data and time steps, (2) default initial condition for three-phase flow simulation, (3) entry of tabulated data for relative permeabilities and capillary pressures, (4) specification of steady-state pressure and flux boundary conditions, (5) computation and printout of Darcy velocity components and saturation for each fluid phase, (6) mass balance computation, and (7) printout control options.

The fifth problem (Section 10.6) was used to show the code's capability and options for simulating solute transport. The exercised options are: (1) automatic generation of mesh data and time steps, (2) default initial condition for transport simulation, (3) use of Darcy velocity and saturation data written on an external file on unit 9 from a previous flow simulation, (4) input of solute transport parameters, (5) specification of the third-type boundary conditions at the inlet nodes, (6) mass balance computation for transport, and (7) printout control options.

10.2 SINGLE-PHASE HYSTERETIC FLOW SIMULATION PROBLEM

10.2.1 Input Data

This problem concerns transient drainage and infiltration in a one-dimensional soil column with hysteresis effects (See Section 4.2.1 for problem description). The input data file is given in Table 10.1. The 60 cm tall soil column is discretized into 60 elements with equal nodal spacings. The initial condition is given in terms of water saturation. It should be noted that the hydraulic conductivity, rather than the intrinsic permeability, is provided in the input file. Normally, SAMFT2D 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 boundary is a prescribed time varying pressure. The time variation is given in input records 15B and 15C.

10.2.2 Output

The main (printer) output file for the transient drainage and infiltration problem with hysteresis is listed in Table 10.2. 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 generated grid data;
- 4) Summary of prescribed boundary conditions and initial values of water pressure and saturation;
- 5) Nonlinear iteration summary for each time step;

Table 10.1. Input data file for the single-phase hysteretic flow simulation problem.

SAMFT2D HYSTERETIC FLOW PROBLEM (CM,MIN) - RESULT IN TERMS OF EFF. SAT.											GROUP 1				
1	2	1	0	1	0	1	200	122	60	1	0	0	1	1	GROUP 2
0	10		0.10		0.005		0.010		1.00		0.000	4	0	GROUP 3	
0	1	0	0	0	20	0	100	0	1	0	0	1	2	GROUP 4	
		0.0	1.0		0.01		5.0		125.0					GROUP 5	
1	2		0.0		0.0									GROUP 6	
1	1		0.0		0.0									GROUP 7A	
2	1		60.0		0.0									GROUP 7B	
		0.000	23.56		0.000		.000		.301		0.00			GROUP 7B	
		1.0	1.0		0.0									GROUP 91A	
		0.0	5.509		0.0306		6.779		0.0		1.0		1.0	GROUP 91B	
		1.0	0.0527										1.0	GROUP 91C	
+1		1.0	1	60	1	1								GROUP 91IA	
61	2		2.0		1.	0	0							GROUP 91IB	
	2.		1.0		2.		60.		1.0		1.00		0.	GROUP 11	
0	2		2	0									0.	GROUP 13	
121	1		0.00E0		0.00E0									GROUP 14	
122	1		0.00E0		0.00E0									GROUP 14B	
1	1	15	0											GROUP 14B	
		0.0	7.27		10.54		22.76		26.20		35.17		45.52	54.90	GROUP 15A
		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	
2	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	
2														GROUP 20A	
1	2													GROUP 20B	
		68.0	125.0											GROUP 22A	

Table 10.2. Output for the single-phase hysteretic flow simulation problem.

THIS OUTPUT GENERATED BY SAMFT2D
INPUT FILE NAME = 2D10-2.DAT

PROBLEM IDENTIFICATION NUMBER = 1
PROBLEM EXECUTION INDEX.....(IEXEC) = 1

PROBLEM TITLE

SAMFT2D HYSTERETIC 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
MATERIAL NUMBER INPUT ? (1=YES,0=NO)(IMNUMR).... = 0
TOTAL NUMBER OF 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 NODES(NP) = 122
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
SEQUENCE OF NODE NUMBERING (0=Y-,1=X-DIR).(ISWAP) = 1

INPUT / OUTPUT CONTROL PARAMETERS

VELOCITY/INPUT.....(NVREAD) = 0
BOUNDARY NODE DATA READ (1=YES, 0=NO)....(IOULT) = 1
NUMBER OF NODES FOR WHICH I.C. ARE READ....(NPIN) = 0
OUTPUT REQUIREMENT INDICATOR:
(0=ALL DATA, 1=NO ELEMENT DATA,
2=NO MESH DATA, 3=NO MESH AND I.C. DATA..(IPRD) = 0
UNIT 9 OUTPUT (1=YES, 0=NO).....(NVWRIT) = 0
VELOCITY PRINTOUT CONTROL INDEX.....(NVPR) = 20
UNIT 10 OUTPUT (0=NONE, N=NTH).....(NPLOT) = 0
NODAL VALUE PRINTOUT CONTROL INDEX.....(NSTEP) = 100
OBSERVATION NODE INDEX.....(IOBSND) = 0
MASS BALANCE TO BE PERFORMED (1=YES,0=NO).(IMBAL) = 1
UNIT 8 OUTPUT (1=YES, 0=NO).....(NOWRIT) = 0
PRINT CHECK OPTION INDEX.....(IPRCHK) = 0
PRESSURE HEAD OUTPUT OPTION INDEX.....(IPWOUT) = 1
OUTPUT SPECIFIED TIME INDEX.....(NPRCON) = 2

MAX. NUMBER OF NONLINEAR FLOW ITERATIONS..(NITMAX) = 10
 EQUIVALENT FRESHWATER HEAD TOLERANCE.....(HTOL) = 0.1000E+00
 SATURATION TOLERANCE.....(STOL) = 0.5000E-02
 GRAVITATIONAL ACCELERATION.....(GCONST) = 0.1000E+01
 ATMOSPHERIC PRESSURE.....(PATM) = 0.0000E+00
 MAXIMUM NUMBER OF TIME STEP REQUIREMENTS..(IRESOL) = 4

HYSTERESIS MODELING OPTION SELECTED ..(IHYST=1)

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) = 0.5000E+01
 FINAL TIME VALUE (TEND) = 0.1250E+03

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.....(NCPOINT) = 2
 DEFAULT VALUE OF INITIAL SATURATION OF THE NON-
 AQUEOUS LIQUID PHASE..... HPDFAL(1) = 0.0000E+00
 DEFAULT VALUE OF INITIAL PRESSURE OF THE AIR
 PHASE.....HIDFAL(2) = 0.0000E+00
 DEPTH FROM SOIL SURFACE TO WATER TABLE..HIDFAL(3) = 0.0000E+00

VERTICAL PROFILE FOR INITIAL FUNCTION

CONTROL POINT #	MATERIAL #	VERT. COOR. (+ UPWARD)	FUNCTION VALUE
1	1	0.0000E+00	0.0000E+00
2	1	60.00	0.0000E+00

HYDRAULIC PROPERTIES OF POROUS MEDIA

MATERIAL NUMBER: 1 (I)

PERMEABILITY COMPONENT Kxx.....(PROP(I,1)) = 0.0000E+00
 PERMEABILITY COMPONENT Kyy.....(PROP(I,2)) = 0.2356E+02
 PERMEABILITY COMPONENT KXY.....(PROP(I,3)) = 0.0000E+00
 POROUS MATRIX COMPRESSIBILITY (PROP(I,4)) = 0.0000E+00
 EFFECTIVE POROSITY..... (PROP(I,5)) = 0.3010E+00
 AIR ENTRY PRESSURE HEAD..... (PROP(I,6)) = 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: 1 (I)

IRREDUCIBLE WETTING PHASE SATURATION.....PROP(1,7) = 0.0000E+00
 EXPONENT INDEX OF REL. PERM. FUNCTION....PROP(1,8) = 0.5509E+01
 COEFF. ALPHA.....PROP(1,9) = 0.3060E-01
 POWER INDEX BETA.....PROP(1,10) = 0.6779E+01
 POWER INDEX GAMMA.....PROP(1,11) = 0.8525E+00
 INTERFACIAL SURFACE TENSION (SIGMA-AW)..PROP(1,12) = 0.1000E+01
 INTERFACIAL SURFACE TENSION (SIGMA-NW)..PROP(1,13) = 0.1000E+01
 INTERFACIAL SURFACE TENSION (SIGMA-AN)..PROP(1,14) = 0.1000E+01

ADDITIONAL DATA FOR HYSTERETIC FLOW SIMULATION

PARAMETERS OF MAIN IMBIBITION CURVE FOR SOIL MATERIAL # (1) : 1

MAX. WATER-PHASE SATURATION.....PROP(1,15)= 0.1000E+01
 COEFF. ALPHA.....PROP(1,16)= 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 SPECIFICATION DATA

NUMBER OF ROWS.....(NROWS) = 61
 NUMBER OF COLUMNS.....(NCOLS) = 2
 MAXIMUM ALLOWABLE X-SPACING.....(DXMAX) = 2.00
 MAXIMUM ALLOWABLE Y-SPACING.....(DYMAX) = 1.00
 INPUT INDICATOR FOR GRIDLINE COORD.....(IXYZRD) = 0
 HORIZONTAL PLANE DOMAIN INDICATOR.....(IHORGR) = 0

 X-INCREMENT OF THE FIRST GRID BLOCK(DX) = 2.000
 Y-INCREMENT OF THE FIRST GRID BLOCK(DY) = 1.000
 MAXIMUM VALUE OF X-COORDINATE(X0) = 2.000
 MAXIMUM VALUE OF Y-COORDINATE(Y0) = 60.000
 X-INCREMENT MULTIPLIER(SCFX) = 1.000
 Y-INCREMENT MULTIPLIER(SCFY) = 1.000
 MINIMUM VALUE OF X-COORDINATE(XSTART) = 0.000
 MINIMUM VALUE OF Y-COORDINATE(YSTART) = 0.000

*** FINITE-ELEMENT MESH NODAL CONNECTIONS ***

(NUMBERING IS COUNTER-CLOCKWISE)

ELEMENT	ELEMENTAL NODE NUMBERING					ELEMENT	ELEMENTAL NODE NUMBERING				
1	1	2	4	3	5	2	3	4	6	5	
3	5	6	8	7	4	7	8	10	9		
5	9	10	12	11	6	11	12	14	13		
7	13	14	16	15	8	15	16	18	17		
9	17	18	20	19	10	19	20	22	21		
11	21	22	24	23	12	23	24	26	25		
13	25	26	28	27	14	27	28	30	29		
15	29	30	32	31	16	31	32	34	33		
17	33	34	36	35	18	35	36	38	37		
19	37	38	40	39	20	39	40	42	41		
21	41	42	44	43	22	43	44	46	45		

23	45	46	48	47	24	47	48	50	49
25	49	50	52	51	26	51	52	54	53
27	53	54	56	55	28	55	56	58	57
29	57	58	60	59	30	59	60	62	61
31	61	62	64	63	32	63	64	66	65
33	65	66	68	67	34	67	68	70	69
35	69	70	72	71	36	71	72	74	73
37	73	74	76	75	38	75	76	78	77
39	77	78	80	79	40	79	80	82	81
41	81	82	84	83	42	83	84	86	85
43	85	86	88	87	44	87	88	90	89
45	89	90	92	91	46	91	92	94	93
47	93	94	96	95	48	95	96	98	97
49	97	98	100	99	50	99	100	102	101
51	101	102	104	103	52	103	104	106	105
53	105	106	108	107	54	107	108	110	109
55	109	110	112	111	56	111	112	114	113
57	113	114	116	115	58	115	116	118	117
59	117	118	120	119	60	119	120	122	121

*** NODAL COORDINATES ***

NODE	X-COOR.	Y-COOR.	NODE	X-COOR.	Y-COOR.
1	0.00	0.00	2	2.00	0.00
3	0.00	1.00	4	2.00	1.00
5	0.00	2.00	6	2.00	2.00
7	0.00	3.00	8	2.00	3.00
9	0.00	4.00	10	2.00	4.00
11	0.00	5.00	12	2.00	5.00
13	0.00	6.00	14	2.00	6.00
15	0.00	7.00	16	2.00	7.00
17	0.00	8.00	18	2.00	8.00
19	0.00	9.00	20	2.00	9.00
21	0.00	10.00	22	2.00	10.00
23	0.00	11.00	24	2.00	11.00
25	0.00	12.00	26	2.00	12.00
27	0.00	13.00	28	2.00	13.00
29	0.00	14.00	30	2.00	14.00
31	0.00	15.00	32	2.00	15.00
33	0.00	16.00	34	2.00	16.00
35	0.00	17.00	36	2.00	17.00
37	0.00	18.00	38	2.00	18.00
39	0.00	19.00	40	2.00	19.00
41	0.00	20.00	42	2.00	20.00
43	0.00	21.00	44	2.00	21.00
45	0.00	22.00	46	2.00	22.00
47	0.00	23.00	48	2.00	23.00
49	0.00	24.00	50	2.00	24.00
51	0.00	25.00	52	2.00	25.00
53	0.00	26.00	54	2.00	26.00
55	0.00	27.00	56	2.00	27.00
57	0.00	28.00	58	2.00	28.00
59	0.00	29.00	60	2.00	29.00
61	0.00	30.00	62	2.00	30.00
63	0.00	31.00	64	2.00	31.00
65	0.00	32.00	66	2.00	32.00
67	0.00	33.00	68	2.00	33.00
69	0.00	34.00	70	2.00	34.00
71	0.00	35.00	72	2.00	35.00
73	0.00	36.00	74	2.00	36.00
75	0.00	37.00	76	2.00	37.00
77	0.00	38.00	78	2.00	38.00
79	0.00	39.00	80	2.00	39.00
81	0.00	40.00	82	2.00	40.00

83	0.00	41.00	84	2.00	41.00
85	0.00	42.00	86	2.00	42.00
87	0.00	43.00	88	2.00	43.00
89	0.00	44.00	90	2.00	44.00
91	0.00	45.00	92	2.00	45.00
93	0.00	46.00	94	2.00	46.00
95	0.00	47.00	96	2.00	47.00
97	0.00	48.00	98	2.00	48.00
99	0.00	49.00	100	2.00	49.00
101	0.00	50.00	102	2.00	50.00
103	0.00	51.00	104	2.00	51.00
105	0.00	52.00	106	2.00	52.00
107	0.00	53.00	108	2.00	53.00
109	0.00	54.00	110	2.00	54.00
111	0.00	55.00	112	2.00	55.00
113	0.00	56.00	114	2.00	56.00
115	0.00	57.00	116	2.00	57.00
117	0.00	58.00	118	2.00	58.00
119	0.00	59.00	120	2.00	59.00
121	0.00	60.00	122	2.00	60.00

BOUNDARY CONDITION DATA

NUMBER OF STEADY DIRICHLET BOUNDARIES (NBTO) = 0
NUMBER OF STEADY FLUX BOUNDARIES (NDFLUX) = 2
NUMBER OF TRANSIENT DIRICHLET BOUNDARIES.... (NBHVAR) = 2
NUMBER OF TRANSIENT FLUX BOUNDARIES.... (NBFVAR) = 0

STEADY-STATE FLUX BOUNDARY CONDITIONS

INDEX	NODE NO.	D.V. NO.	FLUID FLUX VALUE
1	121	1	0.000000E+00
2	122	1	0.000000E+00

TRANSIENT DIRICHLET BOUNDARY CONDITIONS

TIME DEPENDENT DIRICHLET B. C. FOR NODE NO. 1 VALUE OF D.V. NO. 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

TIME DEPENDENT DIRICHLET B. C. FOR NODE NO. 2 VALUE OF D.V. NO. 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

 * INITIAL CONDITION FOR FLOW PROBLEM *

NODE	PRESSURE (Pw)	NODE	PRESSURE (Pw)	NODE	PRESSURE (Pw)	NODE	PRESSURE (Pw)	NODE	PRESSURE (Pw)
1	0.00000E+00	2	0.00000E+00	3	0.00000E+00	4	0.00000E+00	5	0.00000E+00
6	0.00000E+00	7	0.00000E+00	8	0.00000E+00	9	0.00000E+00	10	0.00000E+00
11	0.00000E+00	12	0.00000E+00	13	0.00000E+00	14	0.00000E+00	15	0.00000E+00
16	0.00000E+00	17	0.00000E+00	18	0.00000E+00	19	0.00000E+00	20	0.00000E+00
21	0.00000E+00	22	0.00000E+00	23	0.00000E+00	24	0.00000E+00	25	0.00000E+00
26	0.00000E+00	27	0.00000E+00	28	0.00000E+00	29	0.00000E+00	30	0.00000E+00
31	0.00000E+00	32	0.00000E+00	33	0.00000E+00	34	0.00000E+00	35	0.00000E+00
36	0.00000E+00	37	0.00000E+00	38	0.00000E+00	39	0.00000E+00	40	0.00000E+00
41	0.00000E+00	42	0.00000E+00	43	0.00000E+00	44	0.00000E+00	45	0.00000E+00
46	0.00000E+00	47	0.00000E+00	48	0.00000E+00	49	0.00000E+00	50	0.00000E+00
51	0.00000E+00	52	0.00000E+00	53	0.00000E+00	54	0.00000E+00	55	0.00000E+00
56	0.00000E+00	57	0.00000E+00	58	0.00000E+00	59	0.00000E+00	60	0.00000E+00
61	0.00000E+00	62	0.00000E+00	63	0.00000E+00	64	0.00000E+00	65	0.00000E+00
66	0.00000E+00	67	0.00000E+00	68	0.00000E+00	69	0.00000E+00	70	0.00000E+00
71	0.00000E+00	72	0.00000E+00	73	0.00000E+00	74	0.00000E+00	75	0.00000E+00
76	0.00000E+00	77	0.00000E+00	78	0.00000E+00	79	0.00000E+00	80	0.00000E+00
81	0.00000E+00	82	0.00000E+00	83	0.00000E+00	84	0.00000E+00	85	0.00000E+00
86	0.00000E+00	87	0.00000E+00	88	0.00000E+00	89	0.00000E+00	90	0.00000E+00
91	0.00000E+00	92	0.00000E+00	93	0.00000E+00	94	0.00000E+00	95	0.00000E+00
96	0.00000E+00	97	0.00000E+00	98	0.00000E+00	99	0.00000E+00	100	0.00000E+00
101	0.00000E+00	102	0.00000E+00	103	0.00000E+00	104	0.00000E+00	105	0.00000E+00
106	0.00000E+00	107	0.00000E+00	108	0.00000E+00	109	0.00000E+00	110	0.00000E+00
111	0.00000E+00	112	0.00000E+00	113	0.00000E+00	114	0.00000E+00	115	0.00000E+00
116	0.00000E+00	117	0.00000E+00	118	0.00000E+00	119	0.00000E+00	120	0.00000E+00
121	0.00000E+00	122	0.00000E+00						

ELEM. SATURAT. (Sw) WETTING-DRYING INDEX ELEM. SATURAT. (Sw) WETTING-DRYING INDEX

1	0.10000E+01	1	2	0.10000E+01	1
3	0.10000E+01	1	4	0.10000E+01	1
5	0.10000E+01	1	6	0.10000E+01	1
7	0.10000E+01	1	8	0.10000E+01	1
9	0.10000E+01	1	10	0.10000E+01	1
11	0.10000E+01	1	12	0.10000E+01	1
13	0.10000E+01	1	14	0.10000E+01	1
15	0.10000E+01	1	16	0.10000E+01	1
17	0.10000E+01	1	18	0.10000E+01	1
19	0.10000E+01	1	20	0.10000E+01	1
21	0.10000E+01	1	22	0.10000E+01	1
23	0.10000E+01	1	24	0.10000E+01	1
25	0.10000E+01	1	26	0.10000E+01	1
27	0.10000E+01	1	28	0.10000E+01	1
29	0.10000E+01	1	30	0.10000E+01	1
31	0.10000E+01	1	32	0.10000E+01	1
33	0.10000E+01	1	34	0.10000E+01	1
35	0.10000E+01	1	36	0.10000E+01	1
37	0.10000E+01	1	38	0.10000E+01	1
39	0.10000E+01	1	40	0.10000E+01	1
41	0.10000E+01	1	42	0.10000E+01	1
43	0.10000E+01	1	44	0.10000E+01	1
45	0.10000E+01	1	46	0.10000E+01	1
47	0.10000E+01	1	48	0.10000E+01	1
49	0.10000E+01	1	50	0.10000E+01	1
51	0.10000E+01	1	52	0.10000E+01	1
53	0.10000E+01	1	54	0.10000E+01	1
55	0.10000E+01	1	56	0.10000E+01	1
57	0.10000E+01	1	58	0.10000E+01	1
59	0.10000E+01	1	60	0.10000E+01	1

LIST OF BOUNDARY NODE NUMBERS

 1 2

LIST OF SIMULATION OUTPUT TIME VALUES

 0.6800E+02 0.1250E+03

MATRIX BANDWIDTH REQUIRED IN THIS SIMULATION= 7----

***** BEGIN TRANSIENT CALCULATIONS *****

 *** ELAPSED TIME: 1.000 TIME STEP: 1 TIME STEP SIZE: 0.100E+01 ***

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM ERROR	NODE NUMBER	RELAXATION FACTOR
-----	-----	-----	-----	-----
1	120	57.62	4	1.00
2	0	5.1460E-08	121	1.00

 *** ELAPSED TIME: 2.250 TIME STEP: 2 TIME STEP SIZE: 0.125E+01 ***

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM ERROR	NODE NUMBER	RELAXATION FACTOR
1	120	-1.719	4	1.00
2	0	6.0020E-06	122	1.00

 *** ELAPSED TIME: 3.813 TIME STEP: 3 TIME STEP SIZE: 0.156E+01 ***

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM ERROR	NODE NUMBER	RELAXATION FACTOR
1	120	-2.149	122	1.00
2	0	1.1832E-05	122	1.00

 *** ELAPSED TIME: 5.766 TIME STEP: 4 TIME STEP SIZE: 0.195E+01 ***

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM ERROR	NODE NUMBER	RELAXATION FACTOR
1	120	-2.687	118	1.00
2	0	8.6150E-05	121	1.00

 *** ELAPSED TIME: 8.207 TIME STEP: 5 TIME STEP SIZE: 0.244E+01 ***

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM ERROR	NODE NUMBER	RELAXATION FACTOR
1	120	-4.935	4	1.00
2	0	2.7768E-03	122	1.00

 *** ELAPSED TIME: 11.26 TIME STEP: 6 TIME STEP SIZE: 0.305E+01 ***

NUMBER OF

ITERATION	NON-CONVERGENT NODES	MAXIMUM ERROR	NODE NUMBER	RELAXATION FACTOR
1	120	-7.723	4	1.00
2	0	7.0758E-02	122	0.994

 *** ELAPSED TIME: 15.07 TIME STEP: 7 TIME STEP SIZE: 0.381E+01 ***

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM ERROR	NODE NUMBER	RELAXATION FACTOR
1	120	-3.173	122	1.00
2	0	3.1524E-02	122	0.993

 *** ELAPSED TIME: 19.84 TIME STEP: 8 TIME STEP SIZE: 0.477E+01 ***

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM ERROR	NODE NUMBER	RELAXATION FACTOR
1	120	-3.903	96	1.00
2	0	7.3819E-02	121	0.987

 *** ELAPSED TIME: 24.84 TIME STEP: 9 TIME STEP SIZE: 0.500E+01 ***

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM ERROR	NODE NUMBER	RELAXATION FACTOR
1	120	-8.438	4	1.00
2	94	0.9264	122	0.929
3	0	-6.4362E-02	122	0.951

 *** ELAPSED TIME: 29.84 TIME STEP: 10 TIME STEP SIZE: 0.500E+01 ***

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM ERROR	NODE NUMBER	RELAXATION FACTOR
1	120	-8.027	75	1.00
2	70	3.168	119	0.767
3	26	0.1925	104	1.00
4	0	-1.4830E-02	118	0.950

 *** ELAPSED TIME: 34.84 TIME STEP: 11 TIME STEP SIZE: 0.500E+01 ***

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM ERROR	NODE NUMBER	RELAXATION FACTOR
1	120	-5.773	75	1.00
2	44	0.9691	101	0.894
3	0	-5.9538E-02	122	0.955

 *** ELAPSED TIME: 39.84 TIME STEP: 12 TIME STEP SIZE: 0.500E+01 ***

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM ERROR	NODE NUMBER	RELAXATION FACTOR
1	120	-4.970	61	1.00
2	48	0.7732	91	0.901
3	0	-3.5266E-02	122	0.967

 *** ELAPSED TIME: 44.84 TIME STEP: 13 TIME STEP SIZE: 0.500E+01 ***

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM ERROR	NODE NUMBER	RELAXATION FACTOR
1	120	-4.870	49	1.00
2	44	0.8455	81	0.891
3	0	3.1864E-02	72	1.00

 *** ELAPSED TIME: 49.84 TIME STEP: 14 TIME STEP SIZE: 0.500E+01 ***

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM ERROR	NODE NUMBER	RELAXATION FACTOR
1	120	-5.277	35	1.00
2	36	1.136	71	0.866
3	0	4.8491E-02	62	1.00

 *** ELAPSED TIME: 54.84 TIME STEP: 15 TIME STEP SIZE: 0.500E+01 ***

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM ERROR	NODE NUMBER	RELAXATION FACTOR
1	120	-5.347	27	1.00
2	34	1.139	61	0.867
3	0	4.6781E-02	51	1.00

 *** ELAPSED TIME: 59.84 TIME STEP: 16 TIME STEP SIZE: 0.500E+01 ***

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM ERROR	NODE NUMBER	RELAXATION FACTOR
1	120	-4.800	20	1.00
2	26	0.7727	52	0.898
3	0	2.6586E-02	41	1.00

 *** ELAPSED TIME: 64.84 TIME STEP: 17 TIME STEP SIZE: 0.500E+01 ***

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM ERROR	NODE NUMBER	RELAXATION FACTOR
1	120	-2.124	26	1.00
2	16	-0.1214	51	1.00
3	0	-7.6687E-03	52	1.00

 *** ELAPSED TIME: 69.84 TIME STEP: 18 TIME STEP SIZE: 0.500E+01 ***

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM ERROR	NODE NUMBER	RELAXATION FACTOR
1	120	8.491	4	1.00
2	46	9.759	48	1.00
3	34	-2.860	48	0.822
4	30	-1.781	48	1.00
5	22	-0.8476	47	1.00
6	8	-0.2261	48	1.00
7	0	5.5404E-02	58	0.849

**** ELAPSED SIMULATION TIME : 68.00

*** FLUID FLOW MASS BALANCE INFORMATION AT TIME = 0.6984E+02***

*** MASS BALANCE, FLUID, AND FLOW INFORMATION ***

FLUID PHASE NUMBER 1
 NET FLOW RATE DUE TO BOUNDARY FLUX AND SINKS 4.41371E-01
 RATE OF FLUID ACCUMULATION 4.41467E-01
 MASS BALANCE ERROR -9.59606E-05
 NORMALIZED MASS BALANCE ERROR 1.08696E-04
 CUMULATIVE FLUID STORAGE -2.24518E+01

*** NODAL PRESSURE VALUES ***

NODE	PRESSURE (Pw)	NODE	PRESSURE (Pw)	NODE	PRESSURE (Pw)	NODE	PRESSURE (Pw)	NODE	PRESSURE (Pw)
1	-11.522	2	-11.522	3	-12.526	4	-12.526	5	-13.530
6	-13.530	7	-14.533	8	-14.533	9	-15.537	10	-15.537
11	-16.540	12	-16.540	13	-17.543	14	-17.543	15	-18.546
16	-18.546	17	-19.548	18	-19.548	19	-20.550	20	-20.550
21	-21.550	22	-21.550	23	-22.550	24	-22.550	25	-23.548
26	-23.548	27	-24.544	28	-24.544	29	-25.535	30	-25.535
31	-26.521	32	-26.521	33	-27.499	34	-27.499	35	-28.465
36	-28.465	37	-29.414	38	-29.414	39	-30.340	40	-30.340
41	-31.238	42	-31.238	43	-32.106	44	-32.106	45	-32.941
46	-32.941	47	-33.746	48	-33.746	49	-34.527	50	-34.527
51	-35.284	52	-35.284	53	-36.020	54	-36.020	55	-36.735
56	-36.735	57	-37.409	58	-37.409	59	-38.008	60	-38.008
61	-38.508	62	-38.508	63	-38.901	64	-38.901	65	-39.196
66	-39.196	67	-39.419	68	-39.419	69	-39.592	70	-39.592
71	-39.735	72	-39.735	73	-39.859	74	-39.859	75	-39.974
76	-39.974	77	-40.083	78	-40.083	79	-40.190	80	-40.190
81	-40.296	82	-40.296	83	-40.404	84	-40.404	85	-40.513
86	-40.513	87	-40.624	88	-40.624	89	-40.739	90	-40.739
91	-40.858	92	-40.858	93	-40.981	94	-40.981	95	-41.110
96	-41.110	97	-41.246	98	-41.246	99	-41.389	100	-41.389
101	-41.543	102	-41.543	103	-41.707	104	-41.707	105	-41.885
106	-41.885	107	-42.079	108	-42.079	109	-42.295	110	-42.295
111	-42.537	112	-42.537	113	-42.814	114	-42.814	115	-43.140
116	-43.140	117	-43.538	118	-43.538	119	-44.055	120	-44.055
121	-44.810	122	-44.810						

 *** ELAPSED TIME: 73.84 TIME STEP: 19 TIME STEP SIZE: 0.400E+01 ***

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM ERROR	NODE NUMBER	RELAXATION FACTOR
1	118	7.287	33	1.00

2	34	-0.4616	66	0.959
3	4	-0.1131	66	1.00
4	0	-9.8355E-03	65	1.00

 *** ELAPSED TIME: 77.84 TIME STEP: 20 TIME STEP SIZE: 0.400E+01 ***

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM ERROR	NODE NUMBER	RELAXATION FACTOR
1	118	6.312	66	1.00
2	46	-1.642	66	0.840
3	26	0.1795	79	0.917
4	0	3.9702E-02	79	1.00

*** ELEMENTAL FLUID VELOCITY ***

ELEMENT	X-VELOCITY	Y-VELOCITY	ELEMENT	X-VELOCITY	Y-VELOCITY	ELEMENT	X-VELOCITY	Y-VELOCITY
1	0.000E+00	0.158	2	0.000E+00	0.158	3	0.000E+00	0.158
4	0.000E+00	0.158	5	0.000E+00	0.158	6	0.000E+00	0.158
7	0.000E+00	0.158	8	0.000E+00	0.158	9	0.000E+00	0.158
10	0.000E+00	0.157	11	0.000E+00	0.157	12	0.000E+00	0.157
13	0.000E+00	0.155	14	0.000E+00	0.153	15	0.000E+00	0.150
16	0.000E+00	0.144	17	0.000E+00	0.136	18	0.000E+00	0.126
19	0.000E+00	0.114	20	0.000E+00	0.100	21	0.000E+00	8.705E-02
22	0.000E+00	7.420E-02	23	0.000E+00	6.241E-02	24	0.000E+00	5.191E-02
25	0.000E+00	4.276E-02	26	0.000E+00	3.491E-02	27	0.000E+00	2.827E-02
28	0.000E+00	2.273E-02	29	0.000E+00	1.814E-02	30	0.000E+00	1.435E-02
31	0.000E+00	1.124E-02	32	0.000E+00	8.669E-03	33	0.000E+00	6.502E-03
34	0.000E+00	4.812E-03	35	0.000E+00	3.508E-03	36	0.000E+00	2.536E-03
37	0.000E+00	1.850E-03	38	0.000E+00	1.402E-03	39	0.000E+00	-3.326E-04
40	0.000E+00	-2.828E-03	41	0.000E+00	-4.562E-03	42	0.000E+00	-5.553E-03
43	0.000E+00	-5.593E-03	44	0.000E+00	-5.280E-03	45	0.000E+00	-4.931E-03
46	0.000E+00	-4.570E-03	47	0.000E+00	-4.208E-03	48	0.000E+00	-3.851E-03
49	0.000E+00	-3.500E-03	50	0.000E+00	-3.156E-03	51	0.000E+00	-2.820E-03
52	0.000E+00	-2.491E-03	53	0.000E+00	-2.170E-03	54	0.000E+00	-1.857E-03
55	0.000E+00	-1.552E-03	56	0.000E+00	-1.256E-03	57	0.000E+00	-9.675E-04
58	0.000E+00	-6.875E-04	59	0.000E+00	-4.145E-04	60	0.000E+00	-1.421E-04

 *** ELAPSED TIME: 81.84 TIME STEP: 21 TIME STEP SIZE: 0.400E+01 ***

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM ERROR	NODE NUMBER	RELAXATION FACTOR
1	116	4.716	70	1.00
2	44	-1.099	76	0.856
3	2	0.1025	88	0.930
4	0	-3.4820E-02	86	0.783

 *** ELAPSED TIME: 85.84 TIME STEP: 22 TIME STEP SIZE: 0.400E+01 ***

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM ERROR	NODE NUMBER	RELAXATION FACTOR
1	116	4.202	74	1.00
2	44	-1.036	82	0.848
3	0	8.2981E-02	94	0.939

 *** ELAPSED TIME: 90.84 TIME STEP: 23 TIME STEP SIZE: 0.500E+01 ***

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM ERROR	NODE NUMBER	RELAXATION FACTOR
1	116	4.242	81	1.00
2	44	-1.163	87	0.832
3	0	9.4916E-02	100	0.937

 *** ELAPSED TIME: 95.84 TIME STEP: 24 TIME STEP SIZE: 0.500E+01 ***

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM ERROR	NODE NUMBER	RELAXATION FACTOR
1	118	3.870	88	1.00
2	42	-1.121	96	0.824
3	0	-6.6226E-02	103	1.00

 *** ELAPSED TIME: 100.8 TIME STEP: 25 TIME STEP SIZE: 0.500E+01 ***

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM ERROR	NODE NUMBER	RELAXATION FACTOR
1	118	3.803	89	1.00
2	40	-0.9783	98	0.842
3	0	6.8843E-02	110	0.946

 *** ELAPSED TIME: 105.8 TIME STEP: 26 TIME STEP SIZE: 0.500E+01 ***

NUMBER OF

ITERATION	NON-CONVERGENT NODES	MAXIMUM ERROR	NODE NUMBER	RELAXATION FACTOR
1	116	3.979	96	1.00
2	40	-1.176	104	0.821
3	8	0.1211	114	0.920
4	0	-9.8728E-03	105	0.943

 *** ELAPSED TIME: 110.8 TIME STEP: 27 TIME STEP SIZE: 0.500E+01 ***

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM ERROR	NODE NUMBER	RELAXATION FACTOR
1	116	4.365	102	1.00
2	38	-1.817	110	0.756
3	2	0.1573	118	0.926
4	0	1.5471E-02	118	1.00

 *** ELAPSED TIME: 115.8 TIME STEP: 28 TIME STEP SIZE: 0.500E+01 ***

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM ERROR	NODE NUMBER	RELAXATION FACTOR
1	120	4.962	114	1.00
2	38	-2.533	114	0.709
3	18	0.3476	121	0.879
4	0	5.6153E-02	122	1.00

 *** ELAPSED TIME: 120.8 TIME STEP: 29 TIME STEP SIZE: 0.500E+01 ***

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM ERROR	NODE NUMBER	RELAXATION FACTOR
1	120	9.979	122	1.00
2	34	-7.321	122	0.607
3	26	-2.092	122	1.00
4	16	1.740	122	0.566
5	4	0.2983	121	1.00
6	4	-0.2012	121	0.633
7	0	9.9963E-02	121	0.585

 *** ELAPSED TIME: 124.8 TIME STEP: 30 TIME STEP SIZE: 0.400E+01 ***

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM ERROR	NODE NUMBER	RELAXATION FACTOR
1	120	4.827	121	1.00
2	28	-3.171	121	0.641
3	18	-0.3823	121	1.00
4	8	0.1464	121	0.774
5	0	-1.7876E-02	121	0.900

 *** ELAPSED TIME: 128.8 TIME STEP: 31 TIME STEP SIZE: 0.400E+01 ***

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM ERROR	NODE NUMBER	RELAXATION FACTOR
1	120	5.052	117	1.00
2	24	-2.732	121	0.695
3	10	-0.2739	114	1.00
4	0	7.7051E-02	118	0.829

 **** ELAPSED SIMULATION TIME : 125.0

*** FLUID FLOW MASS BALANCE INFORMATION AT TIME = 0.1288E+03***

*** MASS BALANCE, FLUID, AND FLOW INFORMATION ***

FLUID PHASE NUMBER 1
 NET FLOW RATE DUE TO BOUNDARY FLUX AND SINKS 2.25187E-01
 RATE OF FLUID ACCUMULATION 2.24967E-01
 MASS BALANCE ERROR 2.19676E-04
 NORMALIZED MASS BALANCE ERROR 4.88003E-04
 CUMULATIVE FLUID STORAGE -6.81039E+00

*** NODAL PRESSURE VALUES ***

NODE	PRESSURE (Pw)	NODE	PRESSURE (Pw)	NODE	PRESSURE (Pw)	NODE	PRESSURE (Pw)	NODE	PRESSURE (Pw)
1	27.900	2	27.900	3	26.895	4	26.895	5	25.890
6	25.890	7	24.885	8	24.885	9	23.880	10	23.880
11	22.875	12	22.875	13	21.870	14	21.870	15	20.865
16	20.865	17	19.860	18	19.860	19	18.855	20	18.855
21	17.850	22	17.850	23	16.845	24	16.845	25	15.840
26	15.840	27	14.835	28	14.835	29	13.830	30	13.830
31	12.825	32	12.825	33	11.820	34	11.820	35	10.815

36	10.815	37	9.8097	38	9.8097	39	8.8047	40	8.8047
41	7.7997	42	7.7997	43	6.7947	44	6.7947	45	5.7897
46	5.7897	47	4.7847	48	4.7847	49	3.7797	50	3.7797
51	2.7747	52	2.7747	53	1.7697	54	1.7697	55	0.76470
56	0.76470	57	-0.24030	58	-0.24030	59	-1.2453	60	-1.2453
61	-2.2503	62	-2.2503	63	-3.2553	64	-3.2553	65	-4.2603
66	-4.2603	67	-5.2653	68	-5.2653	69	-6.2703	70	-6.2703
71	-7.2753	72	-7.2753	73	-8.2804	74	-8.2804	75	-9.2854
76	-9.2854	77	-10.291	78	-10.291	79	-11.296	80	-11.296
81	-12.301	82	-12.301	83	-13.307	84	-13.307	85	-14.313
86	-14.313	87	-15.320	88	-15.320	89	-16.329	90	-16.329
91	-17.340	92	-17.340	93	-18.355	94	-18.355	95	-19.378
96	-19.378	97	-20.413	98	-20.413	99	-21.469	100	-21.469
101	-22.558	102	-22.558	103	-23.701	104	-23.701	105	-24.927
106	-24.927	107	-26.269	108	-26.269	109	-27.759	110	-27.759
111	-29.436	112	-29.436	113	-31.281	114	-31.281	115	-33.268
116	-33.268	117	-35.270	118	-35.270	119	-37.130	120	-37.130
121	-38.530	122	-38.530						

***** SAMFT2D HAS SOLVED THE PROBLEM *****

 *** CPU TIME USED: 95.38 SECS. ***

- 6) For each selected output time value:
 - nodal values of pressure head
 - summary of the volumetric flow balance
 - element values of saturation
 - element values of Darcy velocity.
- 7) CPU time for the simulation. Note that the printed value corresponds to execution on a 25 Mhz 80386 computer.

10.3 TWO-PHASE BUCKLEY-LEVERETT FLOW PROBLEM

10.3.1 Input

This example problem is the one-dimensional Buckley-Leverett problem described in Section 4.4.1. The input data file is given in Table 10.3. Note that the capillary effect is neglected by setting the required values on record group 9D to zero. For automatic discretization of the flow domain, 50 elements 102 nodes are specified. There are 4 pressure boundary conditions and 2 flux boundary conditions specified at the right and left hand side boundaries of the flow domain, respectively.

10.3.2 Output

The main output file for the Buckley-Leverett flow problem is listed in Table 10.4. This output file contains the following information:

- 1) Summary of input control parameters;
- 2) List of automatic time step generation parameters;
- 3) List of default initial condition data;
- 4) List of material properties and tabulated constitutive relations;
- 5) Summary of grid specification and boundary condition data;
- 6) Nonlinear iteration summary for each time step;

Table 10.3. Input data file for the Buckley-Leverett problem.

1	1														GROUP 1
TEST FOR SAMFT2D, TWO-PHASE B-L HORIZONL FLOW PROBLEM (IFLOW=3)														GROUP 2	
1	2	2	0	2	0	1	5	102	50	1	1	0	0	0	GROUP 3
1	10		0.01		0.010		0.01000	7.321E10	0.0000E00		4		0		GROUP 4
0	1	0	3	0	5	0	5	0	1	0	0	1	0		GROUP 5
	0.00		2.00E1		1.0		200.00		1.0E20						GROUP 6A
4	2		0.8		0.0		400.0								GROUP 7A
1	1		0.000		0.000000										GROUP 7B
2	1		305.0		0.000000										GROUP 7B
.3000E-12			.3E-12		0.0		0.00E-20		.20		0.0		0.2	0.10	GROUP 9A
1.E03			8.64E01		0.E-20										GROUP 9B
1.E03			8.64E01		0.E-20										GROUP 9B
13	0		0.2		1.0		0.0								GROUP 9D
.2000E00			.0000E00		1.000E00		0.0000E00								GROUP 9D
.2500E00			.6944E-4		0.840200		0.0000E00								GROUP 9D
.3000E00			.0277E00		.6943E00		0.0000E00								GROUP 9D
.3500E00			.0625E00		.5625E00		0.0000E00								GROUP 9D
.4000E00			.1111E00		.4444E00		0.0000E00								GROUP 9D
.4500E00			.1736E00		.3402E00		0.0000E00								GROUP 9D
.5000E00			.2500E00		.2500E00		0.0000E00								GROUP 9D
.5500E00			.3402E00		.1736E00		0.0000E00								GROUP 9D
.6000E00			.4444E00		.1111E00		0.0000E00								GROUP 9D
.6500E00			.5625E00		.0625E00		0.0000E00								GROUP 9D
.7000E00			.6944E00		.0277E00		0.0000E00								GROUP 9D
.7500E00			.8402E00		.6944E-4		0.0000E00								GROUP 9D
.8000E00			1.000E00		.0000E00		0.0000E00								GROUP 9D
2	51		6.10		10.		0	1							GROUP 11
	6.10		10.00		305.		10.0		1.0		1.0		0.0	0.0	GROUP 13
4	2		0		0										GROUP 14
101	1		0.0000E04												GROUP 14B
101	2		0.0000E04												GROUP 14B
102	1		0.0000E04												GROUP 14B
102	2		0.0000E04												GROUP 14B
1	1		0.6500E02												GROUP 14C
2	1		0.6500E02												GROUP 14C
4															GROUP 20A
1	2	101	102												GROUP 20B

Table 10.4. Output for the Buckley-Leverett problem.

 THIS OUTPUT GENERATED BY SAMFT2D
 INPUT FILE NAME = 2D10-3.DAT

PROBLEM IDENTIFICATION NUMBER = 1
 PROBLEM EXECUTION INDEX.....(IEXEC) = 1

PROBLEM TITLE

 TEST FOR SAMFT2D,TWO-PHASE B-L HORIZONL FLOW PROBLEM (IFLOW=3)

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) = 2
 MATERIAL NUMBER INPUT ? (1=YES,0=NO)(IMNUMR).... = 0
 TOTAL NUMBER OF DEPENDENT VARIABLES.....(NVAR) = 2
 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 NODES(NP) = 102
 TOTAL NUMBER OF ELEMENTS(NE) = 50
 NUMBER OF POROUS MATERIALS(NMAT) = 1
 SOIL CONSTITUTIVE DATA(0=FUNCTION,1=TABLE)(KPROP) = 1
 INITIAL CONDITION NON-UNIFORMITY INDEX(NONU) = 0
 SEQUENCE OF NODE NUMBERING (0=Y-,1=X-DIR).(ISWAP) = 0

INPUT / OUTPUT CONTROL PARAMETERS

 VELOCITY/INPUT.....(NVREAD) = 0
 BOUNDARY NODE DATA READ (1=YES, 0=NO)....(IOUTLT) = 1
 NUMBER OF NODES FOR WHICH I.C. ARE READ....(NPIN) = 0
 OUTPUT REQUIREMENT INDICATOR:
 (0=ALL DATA, 1=NO ELEMENT DATA,
 2=NO MESH DATA, 3=NO MESH AND I.C. DATA..(IPRD) = 3
 UNIT 9 OUTPUT (1=YES, 0=NO).....(NVWRIT) = 0
 VELOCITY PRINTOUT CONTROL INDEX.....(NVPR) = 5
 UNIT 10 OUTPUT (0=NONE, N=NTH).....(NPLOT) = 0
 NODAL VALUE PRINTOUT CONTROL INDEX.....(NSTEP) = 5
 OBSERVATION NODE INDEX.....(IOBSND) = 0
 MASS BALANCE TO BE PERFORMED (1=YES,0=NO).(IMBAL) = 1
 UNIT 8 OUTPUT (1=YES, 0=NO).....(NOWRIT) = 0
 PRINT CHECK OPTION INDEX.....(IPRCHK) = 0
 PRESSURE HEAD OUTPUT OPTION INDEX.....(IPWOUT) = 1
 OUTPUT SPECIFIED TIME INDEX.....(NPRCON) = 0

MAX. NUMBER OF NONLINEAR FLOW ITERATIONS..(NITMAX) = 10
 EQUIVALENT FRESHWATER HEAD TOLERANCE.....(HTOL) = 0.1000E-01
 SATURATION TOLERANCE.....(STOL) = 0.1000E-01
 GRAVITATIONAL ACCELERATION.....(GCONST) = 0.7321E+11
 ATMOSPHERIC PRESSURE.....(PATM) = 0.0000E+00
 MAXIMUM NUMBER OF TIME STEP REQUIREMENTS..(IRESOL) = 4

TEMPORAL DISCRETIZATION DATA

 INITIAL TIME VALUE (TIMA) = 0.0000E+00
 VALUE OF FIRST TIME STEP (TIN) = 0.2000E+02
 MINIMUM TIME STEP SIZE..... (TMIN) = 0.1000E+01
 MAXIMUM TIME STEP SIZE (TMAX) = 0.2000E+03
 FINAL TIME VALUE (TEND) = 0.1000E+21

DEFAULT INITIAL CONDITION DATA FOR FLOW PROBLEM

 INITIAL CONDITION IDENTIFIER.....(IDFVAR) = 4
 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..... HFDAL(1) = 0.8000E+00
 DEFAULT VALUE OF INITIAL PRESSURE OF THE AIR
 PHASE.....HIDFAL(2) = 0.0000E+00
 DEPTH FROM SOIL SURFACE TO WATER TABLE..HIDFAL(3) = 0.4000E+03

HORIZONTAL PROFILE FOR INITIAL FUNCTION

CONTROL POINT #	MATERIAL #	HORI. COOR. (+ X-CORD)	FUNCTION VALUE
1	1	0.0000E+00	0.0000E+00
2	1	305.0	0.0000E+00

HYDRAULIC PROPERTIES OF POROUS MEDIA

MATERIAL NUMBER: 1 (I)

PERMEABILITY COMPONENT Kxx.....(PROP(I,1)) = 0.3000E-12
 PERMEABILITY COMPONENT Kyy.....(PROP(I,2)) = 0.3000E-12
 PERMEABILITY COMPONENT KXY.....(PROP(I,3)) = 0.0000E+00
 POROUS MATRIX COMPRESSIBILITY (PROP(I,4)) = 0.0000E+00
 EFFECTIVE POROSITY..... (PROP(I,5)) = 0.2000E+00
 AIR ENTRY PRESSURE HEAD..... (PROP(I,6)) = 0.0000E+00

IRREDUCIBLE NAPL SATURATIONSNIRWN(I)= 0.2000E+00
 CRITICAL NAPL SATURATION.....SNSTR(I)= 0.1000E+00

FLUID PROPERTIES

FLUID PHASE NUMBER: 1

REFERENCE DENSITY..... = 0.1000E+04
 REFERENCE DYNAMIC VISCOSITY..... = 0.8640E+02
 COMPRESSIBILITY = 0.0000E+00

FLUID PHASE NUMBER: 2

REFERENCE DENSITY..... = 0.1000E+04

REFERENCE DYNAMIC VISCOSITY..... = 0.8640E+02
 COMPRESSIBILITY = 0.0000E+00

FLUID RETENTION DATA FOR SOIL MATERIAL NO. 1
 =====

IRREDUCIBLE WETTING-PHASE SATURATIONPROP(1,7)= 0.2000E+00
 NAPL REL. PERM. AT Swr.....AKSTAR(I)= 0.1000E+01
 N-W CAPILLARY PRESSURE @ Sw=1.....PCNSW1(I)= 0.0000E+00

TABULATED REL. PERM. AND CAP. PRESSURE DATA FOR SOIL MATERIAL NO. 1

NO. OF ROW ENTRIES FOR PHASE 1 VS. 2 RELATIONSHIPS.= 13

SATURATION - PH1	REL. PERM. - PH1	REL. PERM. - PH21	CAP. PRESSURE - PH21
0.2000E+00	0.0000E+00	0.1000E+01	0.0000E+00
0.2500E+00	0.6944E-04	0.8402E+00	0.0000E+00
0.3000E+00	0.2770E-01	0.6943E+00	0.0000E+00
0.3500E+00	0.6250E-01	0.5625E+00	0.0000E+00
0.4000E+00	0.1111E+00	0.4444E+00	0.0000E+00
0.4500E+00	0.1736E+00	0.3402E+00	0.0000E+00
0.5000E+00	0.2500E+00	0.2500E+00	0.0000E+00
0.5500E+00	0.3402E+00	0.1736E+00	0.0000E+00
0.6000E+00	0.4444E+00	0.1111E+00	0.0000E+00
0.6500E+00	0.5625E+00	0.6250E-01	0.0000E+00
0.7000E+00	0.6944E+00	0.2770E-01	0.0000E+00
0.7500E+00	0.8402E+00	0.6944E-04	0.0000E+00
0.8000E+00	0.1000E+01	0.0000E+00	0.0000E+00

GRID SPECIFICATION DATA

NUMBER OF ROWS.....(NROWS) = 2
 NUMBER OF COLUMNS.....(NCOLS) = 51
 MAXIMUM ALLOWABLE X-SPACING.....(DXMAX) = 6.10
 MAXIMUM ALLOWABLE Y-SPACING.....(DYMAX) = 10.00
 INPUT INDICATOR FOR GRIDLINE COORD.....(IXYZRD) = 0
 HORIZONTAL PLANE DOMAIN INDICATOR.....(IHORGR) = 1

HORIZONTAL PLANE GRID IS USED, THUS GRAVITY TERM OF FLOW EQ. WILL BE NEGLECTED

X-INCREMENT OF THE FIRST GRID BLOCK(DX) = 6.100
 Y-INCREMENT OF THE FIRST GRID BLOCK(DY) = 10.000
 MAXIMUM VALUE OF X-COORDINATE(XO) = 305.000
 MAXIMUM VALUE OF Y-COORDINATE(YO) = 10.000
 X-INCREMENT MULTIPLIER(SCFX) = 1.000
 Y-INCREMENT MULTIPLIER(SCFY) = 1.000
 MINIMUM VALUE OF X-COORDINATE(XSTART) = 0.000
 MINIMUM VALUE OF Y-COORDINATE(YSTART) = 0.000

BOUNDARY CONDITION DATA

NUMBER OF STEADY DIRICHLET BOUNDARIES (NBTO) = 4
 NUMBER OF STEADY FLUX BOUNDARIES (NDFLUX) = 2
 NUMBER OF TRANSIENT DIRICHLET BOUNDARIES.... (NBHVAR) = 0
 NUMBER OF TRANSIENT FLUX BOUNDARIES..... (NBFVAR) = 0

STEADY-STATE DIRICHLET BOUNDARY CONDITIONS

INDEX	NODE NO.	D.V. NO.	PRESCRIBED VALUE	B.C. IDENTIFIER
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1	101	1	0.000000E+00	0
2	101	2	0.000000E+00	0
3	102	1	0.000000E+00	0
4	102	2	0.000000E+00	0

 STEADY-STATE FLUX BOUNDARY CONDITIONS

INDEX	NODE NO.	D.V. NO.	FLUID FLUX VALUE
1	1	1	65.0000
2	2	1	65.0000

 LIST OF BOUNDARY NODE NUMBERS

1 2 101 102

DISTANCE SCALE FACTOR FOR PRESSURE B.C. INCORPORATION = 0.12200E+01

MATRIX BANDWIDTH REQUIRED FOR FLOW SIMULATION = 15
 =====

+++++ BEGIN TRANSIENT CALCULATIONS +++++

 *** ELAPSED TIME: 20.00 TIME STEP: 1 TIME STEP SIZE: 0.200E+02 ***

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM HEAD ERROR	NODE NUMBER	MAXIMUM SATUR. ERROR	NODE NUMBER	RELAXATION FACTOR
1	104	15.81	1	0.426	1	0.469
2	106	8.691	1	0.110	2	1.00
3	8	0.1143	2	0.476E-01	1	1.00
4	2	-0.2520E-01	2	0.137E-02	1	0.863
5	0	-0.2711E-02	2	0.276E-03	3	1.00

 *** ELAPSED TIME: 32.35 TIME STEP: 2 TIME STEP SIZE: 0.123E+02 ***

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM HEAD ERROR	NODE NUMBER	MAXIMUM SATUR. ERROR	NODE NUMBER	RELAXATION FACTOR
1	12	0.1364	1	0.883E-01	2	1.00
2	2	-0.2613E-01	1	0.317E-02	5	0.880

3 0 0.8837E-02 3 0.869E-03 6 0.773

 *** ELAPSED TIME: 60.48 TIME STEP: 3 TIME STEP SIZE: 0.281E+02 ***

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM HEAD ERROR	NODE NUMBER	MAXIMUM SATUR. ERROR	NODE NUMBER	RELAXATION FACTOR
1	12	0.2908	4	0.151	4	1.00
2	12	0.2916E-01	6	0.211E-01	4	1.00
3	4	-0.1125E-01	3	0.904E-03	3	0.772
4	4	-0.1152E-01	3	0.567E-03	3	1.00
5	0	0.7470E-02	3	0.353E-03	4	0.644

 *** ELAPSED TIME: 104.0 TIME STEP: 4 TIME STEP SIZE: 0.436E+02 ***

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM HEAD ERROR	NODE NUMBER	MAXIMUM SATUR. ERROR	NODE NUMBER	RELAXATION FACTOR
1	16	0.4746	4	0.198	5	1.00
2	16	-0.1277	2	0.526E-01	9	0.835
3	12	0.2488E-01	8	0.121E-01	5	0.856
4	0	-0.3826E-02	2	0.214E-02	5	0.887

 *** ELAPSED TIME: 162.9 TIME STEP: 5 TIME STEP SIZE: 0.589E+02 ***

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM HEAD ERROR	NODE NUMBER	MAXIMUM SATUR. ERROR	NODE NUMBER	RELAXATION FACTOR
1	24	0.5357	6	0.198	9	1.00
2	20	0.9609E-01	9	0.349E-01	9	1.00
3	10	-0.1231E-01	8	0.406E-02	14	0.918
4	0	-0.5343E-02	8	0.411E-03	14	1.00

*** NODAL FLUID FLUX VALUES ***

NODAL FLUXES FOR FLUID PHASE # 1

NODE	FLUID FLUX	NODE	FLUID FLUX	NODE	FLUID FLUX	NODE	FLUID FLUX	NODE	FLUID FLUX
1	65.00	2	65.00	101	0.0000E+00	102	0.0000E+00		

.....
 SUM OF ABOVE FLUX VALUES = 130.00

NODAL FLUXES FOR FLUID PHASE # 2

NODE	FLUID FLUX	NODE	FLUID FLUX	NODE	FLUID FLUX	NODE	FLUID FLUX	NODE	FLUID FLUX
1	1.1121E-04	2	1.1121E-04	101	-65.00	102	-65.00		

.....
 SUM OF ABOVE FLUX VALUES = -130.00

*** NODAL PRESSURE VALUES ***

NODE	PRESSURE (Pw)	NODE	PRESSURE (Pw)	NODE	PRESSURE (Pw)	NODE	PRESSURE (Pw)	NODE	PRESSURE (Pw)
1	1.25447E+15	2	1.25447E+15	3	1.22437E+15	4	1.22437E+15	5	1.18678E+15
6	1.18678E+15	7	1.14383E+15	8	1.14383E+15	9	1.09816E+15	10	1.09816E+15
11	1.05666E+15	12	1.05666E+15	13	1.02344E+15	14	1.02344E+15	15	9.97398E+14
16	9.97398E+14	17	9.74557E+14	18	9.74557E+14	19	9.51719E+14	20	9.51719E+14
21	9.28880E+14	22	9.28880E+14	23	9.06042E+14	24	9.06042E+14	25	8.83203E+14
26	8.83203E+14	27	8.60365E+14	28	8.60365E+14	29	8.37527E+14	30	8.37527E+14
31	8.14688E+14	32	8.14688E+14	33	7.91850E+14	34	7.91850E+14	35	7.69011E+14
36	7.69011E+14	37	7.46173E+14	38	7.46173E+14	39	7.23335E+14	40	7.23335E+14
41	7.00496E+14	42	7.00496E+14	43	6.77658E+14	44	6.77658E+14	45	6.54819E+14
46	6.54819E+14	47	6.31981E+14	48	6.31981E+14	49	6.09143E+14	50	6.09143E+14
51	5.86304E+14	52	5.86304E+14	53	5.63466E+14	54	5.63466E+14	55	5.40627E+14
56	5.40627E+14	57	5.17789E+14	58	5.17789E+14	59	4.94951E+14	60	4.94951E+14
61	4.72112E+14	62	4.72112E+14	63	4.49274E+14	64	4.49274E+14	65	4.26435E+14
66	4.26435E+14	67	4.03597E+14	68	4.03597E+14	69	3.80759E+14	70	3.80759E+14
71	3.57920E+14	72	3.57920E+14	73	3.35082E+14	74	3.35082E+14	75	3.12243E+14
76	3.12243E+14	77	2.89405E+14	78	2.89405E+14	79	2.66567E+14	80	2.66567E+14
81	2.43728E+14	82	2.43728E+14	83	2.20890E+14	84	2.20890E+14	85	1.98051E+14
86	1.98051E+14	87	1.75213E+14	88	1.75213E+14	89	1.52375E+14	90	1.52375E+14
91	1.29536E+14	92	1.29536E+14	93	1.06698E+14	94	1.06698E+14	95	8.38595E+13
96	8.38595E+13	97	6.10211E+13	98	6.10211E+13	99	3.81827E+13	100	3.81827E+13
101	1.53443E+13	102	1.53443E+13						

*** NODAL VALUES OF WATER SATURATION ***

NODE	SATURAT. (Sw)	NODE	SATURAT. (Sw)	NODE	SATURAT. (Sw)	NODE	SATURAT. (Sw)	NODE	SATURAT. (Sw)
1	0.71555	2	0.71555	3	0.63748	4	0.63748	5	0.57155
6	0.57155	7	0.50028	8	0.50028	9	0.41615	10	0.41615
11	0.31699	12	0.31699	13	0.23610	14	0.23610	15	0.20003
16	0.20003	17	0.20000	18	0.20000	19	0.20000	20	0.20000
21	0.20000	22	0.20000	23	0.20000	24	0.20000	25	0.20000
26	0.20000	27	0.20000	28	0.20000	29	0.20000	30	0.20000
31	0.20000	32	0.20000	33	0.20000	34	0.20000	35	0.20000
36	0.20000	37	0.20000	38	0.20000	39	0.20000	40	0.20000
41	0.20000	42	0.20000	43	0.20000	44	0.20000	45	0.20000

46	0.20000	47	0.20000	48	0.20000	49	0.20000	50	0.20000
51	0.20000	52	0.20000	53	0.20000	54	0.20000	55	0.20000
56	0.20000	57	0.20000	58	0.20000	59	0.20000	60	0.20000
61	0.20000	62	0.20000	63	0.20000	64	0.20000	65	0.20000
66	0.20000	67	0.20000	68	0.20000	69	0.20000	70	0.20000
71	0.20000	72	0.20000	73	0.20000	74	0.20000	75	0.20000
76	0.20000	77	0.20000	78	0.20000	79	0.20000	80	0.20000
81	0.20000	82	0.20000	83	0.20000	84	0.20000	85	0.20000
86	0.20000	87	0.20000	88	0.20000	89	0.20000	90	0.20000
91	0.20000	92	0.20000	93	0.20000	94	0.20000	95	0.20000
96	0.20000	97	0.20000	98	0.20000	99	0.20000	100	0.20000
101	0.20000	102	0.20000						

*** NODAL VALUES OF NAPL SATURATION ***

NODE	SATURAT. (Sn)	NODE	SATURAT. (Sn)	NODE	SATURAT. (Sn)	NODE	SATURAT. (Sn)	NODE	SATURAT. (Sn)
1	0.28445	2	0.28445	3	0.36252	4	0.36252	5	0.42845
6	0.42845	7	0.49972	8	0.49972	9	0.58385	10	0.58385
11	0.68301	12	0.68301	13	0.76390	14	0.76390	15	0.79997
16	0.79997	17	0.80000	18	0.80000	19	0.80000	20	0.80000
21	0.80000	22	0.80000	23	0.80000	24	0.80000	25	0.80000
26	0.80000	27	0.80000	28	0.80000	29	0.80000	30	0.80000
31	0.80000	32	0.80000	33	0.80000	34	0.80000	35	0.80000
36	0.80000	37	0.80000	38	0.80000	39	0.80000	40	0.80000
41	0.80000	42	0.80000	43	0.80000	44	0.80000	45	0.80000
46	0.80000	47	0.80000	48	0.80000	49	0.80000	50	0.80000
51	0.80000	52	0.80000	53	0.80000	54	0.80000	55	0.80000
56	0.80000	57	0.80000	58	0.80000	59	0.80000	60	0.80000
61	0.80000	62	0.80000	63	0.80000	64	0.80000	65	0.80000
66	0.80000	67	0.80000	68	0.80000	69	0.80000	70	0.80000
71	0.80000	72	0.80000	73	0.80000	74	0.80000	75	0.80000
76	0.80000	77	0.80000	78	0.80000	79	0.80000	80	0.80000
81	0.80000	82	0.80000	83	0.80000	84	0.80000	85	0.80000
86	0.80000	87	0.80000	88	0.80000	89	0.80000	90	0.80000
91	0.80000	92	0.80000	93	0.80000	94	0.80000	95	0.80000
96	0.80000	97	0.80000	98	0.80000	99	0.80000	100	0.80000
101	0.80000	102	0.80000						

*** ELEMENT SATURATION VALUES ***

ELEMENT	PH1-SATUR.	PH2-SATUR.	ELEMENT	PH1-SATUR.	PH2-SATUR.	ELEMENT	PH1-SATUR.	PH2-SATUR.
1	0.677	0.323	2	0.605	0.395	3	0.536	0.464
4	0.458	0.542	5	0.367	0.633	6	0.277	0.723
7	0.218	0.782	8	0.200	0.800	9	0.200	0.800
10	0.200	0.800	11	0.200	0.800	12	0.200	0.800
13	0.200	0.800	14	0.200	0.800	15	0.200	0.800
16	0.200	0.800	17	0.200	0.800	18	0.200	0.800
19	0.200	0.800	20	0.200	0.800	21	0.200	0.800
22	0.200	0.800	23	0.200	0.800	24	0.200	0.800
25	0.200	0.800	26	0.200	0.800	27	0.200	0.800
28	0.200	0.800	29	0.200	0.800	30	0.200	0.800
31	0.200	0.800	32	0.200	0.800	33	0.200	0.800
34	0.200	0.800	35	0.200	0.800	36	0.200	0.800
37	0.200	0.800	38	0.200	0.800	39	0.200	0.800
40	0.200	0.800	41	0.200	0.800	42	0.200	0.800
43	0.200	0.800	44	0.200	0.800	45	0.200	0.800
46	0.200	0.800	47	0.200	0.800	48	0.200	0.800
49	0.200	0.800	50	0.200	0.800			

*** ELEMENTAL FLUID VELOCITIES ***

ELEMENT	X-VELOCITY(PH1)	Y-VELOCITY(PH1)	X-VELOCITY(PH2)	Y-VELOCITY(PH2)
1	0.1267E-01	0.0000E+00	0.3273E-03	0.0000E+00
2	0.1140E-01	0.0000E+00	0.1598E-02	0.0000E+00
3	0.9415E-02	0.0000E+00	0.3585E-02	0.0000E+00
4	0.6512E-02	0.1724E-16	0.6488E-02	0.2982E-16
5	0.3102E-02	-0.4628E-16	0.9704E-02	-0.2873E-15
6	0.7473E-03	-0.3038E-16	0.1228E-01	-0.1178E-14
7	0.7434E-06	-0.9291E-19	0.1312E-01	-0.3489E-14
8	0.5685E-09	-0.5035E-22	0.1300E-01	-0.2303E-14
9	0.0000E+00	0.0000E+00	0.1300E-01	0.4516E-15
10	0.0000E+00	0.5848E-33	0.1300E-01	0.3612E-15
11	0.4209E-19	0.5848E-33	0.1300E-01	0.3612E-15
12	0.0000E+00	0.0000E+00	0.1300E-01	0.0000E+00
13	0.0000E+00	0.0000E+00	0.1300E-01	0.2258E-14
14	0.0000E+00	0.0000E+00	0.1300E-01	0.7225E-15
15	0.0000E+00	0.0000E+00	0.1300E-01	-0.1400E-14
16	0.0000E+00	0.0000E+00	0.1300E-01	0.1355E-15
17	0.0000E+00	0.0000E+00	0.1300E-01	0.2709E-15
18	0.0000E+00	0.0000E+00	0.1300E-01	0.2709E-15
19	0.0000E+00	0.0000E+00	0.1300E-01	0.3522E-14
20	0.0000E+00	0.0000E+00	0.1300E-01	0.5419E-14
21	0.0000E+00	0.0000E+00	0.1300E-01	0.1761E-14
22	0.0000E+00	0.0000E+00	0.1300E-01	0.9483E-15
23	0.0000E+00	0.0000E+00	0.1300E-01	0.7225E-15
24	0.0000E+00	0.0000E+00	0.1300E-01	-0.2258E-15
25	0.0000E+00	0.0000E+00	0.1300E-01	0.1806E-15
26	0.0000E+00	0.0000E+00	0.1300E-01	0.4516E-16
27	0.0000E+00	0.0000E+00	0.1300E-01	0.0000E+00
28	0.0000E+00	0.0000E+00	0.1300E-01	-0.4064E-15
29	0.0000E+00	0.0000E+00	0.1300E-01	0.4516E-15
30	0.0000E+00	0.0000E+00	0.1300E-01	0.5419E-15
31	0.0000E+00	0.0000E+00	0.1300E-01	-0.2709E-15
32	0.0000E+00	0.0000E+00	0.1300E-01	0.1016E-14
33	0.0000E+00	0.0000E+00	0.1300E-01	0.1490E-14
34	0.0000E+00	0.0000E+00	0.1300E-01	0.1355E-14
35	0.0000E+00	0.0000E+00	0.1300E-01	0.7902E-15
36	0.0000E+00	0.0000E+00	0.1300E-01	-0.1535E-14
37	0.0000E+00	0.0000E+00	0.1300E-01	-0.3003E-14
38	0.0000E+00	0.0000E+00	0.1300E-01	-0.1535E-14
39	0.0000E+00	0.0000E+00	0.1300E-01	0.1468E-15
40	0.0000E+00	0.0000E+00	0.1300E-01	0.2935E-15
41	0.0000E+00	0.0000E+00	0.1300E-01	0.5532E-15
42	0.0000E+00	0.0000E+00	0.1300E-01	0.1468E-15
43	0.0000E+00	0.0000E+00	0.1300E-01	-0.5644E-15
44	0.0000E+00	0.0000E+00	0.1300E-01	-0.2935E-15
45	0.0000E+00	0.0000E+00	0.1300E-01	-0.1976E-15
46	0.0000E+00	0.0000E+00	0.1300E-01	-0.2371E-15
47	0.0000E+00	0.0000E+00	0.1300E-01	0.1355E-15
48	0.0000E+00	0.0000E+00	0.1300E-01	0.3104E-15
49	0.0000E+00	0.0000E+00	0.1300E-01	0.1101E-15
50	0.0000E+00	0.0000E+00	0.1300E-01	0.7056E-17

*** FLUID FLOW MASS BALANCE INFORMATION AT TIME = 0.1629E+03***

*** MASS BALANCE, FLUID, AND FLOW INFORMATION ***

FLUID PHASE NUMBER	1
NET FLOW RATE DUE TO BOUNDARY FLUX AND SINKS	1.30000E+02
RATE OF FLUID ACCUMULATION	1.30000E+02
MASS BALANCE ERROR	1.93268E-12
NORMALIZED MASS BALANCE ERROR	7.43337E-15

CUMULATIVE FLUID STORAGE 2.11834E+04

*** MASS BALANCE, FLUID, AND FLOW INFORMATION ***

FLUID PHASE NUMBER 2
NET FLOW RATE DUE TO BOUNDARY FLUX AND SINKS -1.30000E+02
RATE OF FLUID ACCUMULATION -1.30000E+02
MASS BALANCE ERROR 2.22417E-04
NORMALIZED MASS BALANCE ERROR 8.55449E-07
CUMULATIVE FLUID STORAGE -2.11834E+04

***** SAMFT2D HAS SOLVED THE PROBLEM *****

*** CPU TIME USED: 33.90 SECS. ***

- 7) For each selected output time value:
 - nodal values of water pressure
 - nodal values of water and NAPL saturations
 - element saturation values and Darcy velocities
 - summary of mass balance information.
- 8) CPU time for the simulation.

10.4 TWO-PHASE FLOW IN A THREE-PHASE SYSTEM

10.4.1 Input Data

This problem concerns vertical flow of water and NAPL in a partially saturated soil column (see Section 4.4.3 for problem description). The input data file is given in Table 10.5. Note that the relative permeability and capillary pressure data is specified in a tabular form. For automatic discretization of the flow domain, 20 elements and 42 nodes are specified. There are 4 pressure boundary conditions prescribed at the bottom nodes where the fluids are expected to leave the flow system. Additionally, there are 4 flux boundary conditions prescribed at the top nodes where water and NAPL injection occur.

10.4.2 Output

The main output file for the vertical two-phase flow problem is given in Table 10.6, which, unlike all the other output files, was generated using the MIPS computer. This output file contains the following information:

- 1) Summary of input control parameters;
- 2) List of automatic time step generation parameters;
- 3) List of default initial condition data;
- 4) List of material properties and tabulated constitutive relations;

Table 10.5. Input data file for the problem of two-phase flow in a three-phase system.

1	1																			GROUP 1
TEST FOR SAMFT2D, 2-PH FLOW IN A 3-PH SYSTEM WITH 20-ELEMENTS (IFLOW=2)																				
1	3	2	0	2	0	1	20	42	20	1	1	0	1	0	0					GROUP 2
1	10		1.E-2		1.E-2		0.01000		9.8066E0		1.000E05		5		0					GROUP 3
0	1	0	0	0	0	0	10	0	1	0	0	1	0							GROUP 4
	0.0		1.00E03		10.0		8.6400E5		1.00E15											GROUP 5
3	3		0.0		1.00000E5		1.5													GROUP 6A
1	1		0.00		1.000E0															GROUP 7A
2	1		3.50		1.000E0															GROUP 7B
3	1		4.8750		0.850E0															GROUP 7B
0.000E-12	1.0E-12				0.0		1.00E-10		.30		0.0		0.1		0.10					GROUP 7B
1.E03	1.00E-3				1.0E-9															GROUP 9A
9.50E02	1.00E-3				1.0E-9															GROUP 9B
9	9		0.2		.68		.00													GROUP 9B
.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		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
21	2		1.00		.250		0		0											GROUP 11
	1.0		.25		1.0		5.0		1.0		1.0		0.0		0.0					GROUP 13
4	4		0		0															GROUP 14
1	1		1.500E+05		-1															GROUP 14B
1	2		1.500E+05		-1															GROUP 14B
2	1		1.500E+05		-1															GROUP 14B
2	2		1.500E+05		-1															GROUP 14B
41	1		1.5850E-6																	GROUP 14C
41	2		1.4269E-5																	GROUP 14C
42	1		1.5850E-6																	GROUP 14C
42	2		1.4269E-5																	GROUP 14C
4																				GROUP 20A
1	2		41		42															GROUP 20B

Table 10.6. Output for the problem of two-phase flow in a three-phase system.

THIS OUTPUT GENERATED BY SAMFT2D
 INPUT FILE NAME = 2d10-4c.dat

PROBLEM IDENTIFICATION NUMBER = 1
 PROBLEM EXECUTION INDEX.....(IEXEC) = 1

PROBLEM TITLE

 TEST FOR SAMFT2D,2-PH FLOW IN A 3-PH SYSTEM WITH 20-ELEMETS (IFLOW=2)

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) = 2
 MATERIAL NUMBER INPUT ? (1=YES,0=NO)(IMNUMR).... = 0
 TOTAL NUMBER OF DEPENDENT VARIABLES.....(NVAR) = 2
 STEADY STATE SIMULATION(1=YES, 0=NO).....(ISSTA) = 0
 TIME STEP GENERATION INDEX (1=YES, 0=NO) .(ITSGN) = 1
 NUMBER OF TIME STEPS(NTS) = 20
 TOTAL NUMBER OF NODES(NP) = 42
 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) = 0
 SEQUENCE OF NODE NUMBERING (0=Y-,1=X-DIR).(ISWAP) = 1

INPUT / OUTPUT CONTROL PARAMETERS

 VELOCITY/INPUT.....(NVREAD) = 0
 BOUNDARY NODE DATA READ (1=YES, 0=NO).....(IOUTLT) = 1
 NUMBER OF NODES FOR WHICH I.C. ARE READ....(NPIN) = 0
 OUTPUT REQUIREMENT INDICATOR:
 (0=ALL DATA, 1=NO ELEMENT DATA,
 2=NO MESH DATA, 3=NO MESH AND I.C. DATA..(IPRD) = 0
 UNIT 9 OUTPUT (1=YES, 0=NO).....(NVWRIT) = 0
 VELOCITY PRINTOUT CONTROL INDEX.....(NVPR) = 0
 UNIT 10 OUTPUT (0=NONE, N=NTH).....(NPLOT) = 0
 NODAL VALUE PRINTOUT CONTROL INDEX.....(NSTEP) = 10
 OBSERVATION NODE INDEX.....(IOBSND) = 0
 MASS BALANCE TO BE PERFORMED (1=YES,0=NO).(IMBAL) = 1
 UNIT 8 OUTPUT (1=YES, 0=NO).....(NOWRIT) = 0
 PRINT CHECK OPTION INDEX.....(IPRCHK) = 0
 PRESSURE HEAD OUTPUT OPTION INDEX.....(IPWOUT) = 1
 OUTPUT SPECIFIED TIME INDEX.....(NPRCON) = 0

MAX. NUMBER OF NONLINEAR FLOW ITERATIONS..(NITMAX) = 10
 EQUIVALENT FRESHWATER HEAD TOLERANCE.....(HTOL) = 0.1000E-01
 SATURATION TOLERANCE.....(STOL) = 0.1000E-01
 GRAVITATIONAL ACCELERATION.....(GCONST) = 0.9807E+01
 ATMOSPHERIC PRESSURE.....(PATM) = 0.1000E+06
 MAXIMUM NUMBER OF TIME STEP REQUIREMENTS..(IRESOL) = 5

TEMPORAL DISCRETIZATION DATA

 INITIAL TIME VALUE (TIMA) = 0.0000E+00
 VALUE OF FIRST TIME STEP (TIN) = 0.1000E+04
 MINIMUM TIME STEP SIZE..... (TMIN) = 0.1000E+02
 MAXIMUM TIME STEP SIZE (TMAX) = 0.8640E+06
 FINAL TIME VALUE (TEND) = 0.1000E+16

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) = 3
 DEFAULT VALUE OF INITIAL SATURATION OF THE NON-
 AQUEOUS LIQUID PHASE..... HFDAL(1) = 0.0000E+00
 DEFAULT VALUE OF INITIAL PRESSURE OF THE AIR
 PHASE.....HIDFAL(2) = 0.1000E+06
 DEPTH FROM SOIL SURFACE TO WATER TABLE..HIDFAL(3) = 0.1500E+01

VERTICAL PROFILE FOR INITIAL FUNCTION

CONTROL POINT #	MATERIAL #	VERT. COOR. (+ UPWARD)	FUNCTION VALUE
1	1	0.0000E+00	1.000
2	1	3.500	1.000
3	1	4.875	0.8500

HYDRAULIC PROPERTIES OF POROUS MEDIA

MATERIAL NUMBER: 1 (I)

PERMEABILITY COMPONENT Kxx.....(PROP(I,1)) = 0.0000E+00
 PERMEABILITY COMPONENT Kyy.....(PROP(I,2)) = 0.1000E-11
 PERMEABILITY COMPONENT KXY.....(PROP(I,3)) = 0.0000E+00
 POROUS MATRIX COMPRESSIBILITY (PROP(I,4)) = 0.1000E-09
 EFFECTIVE POROSITY..... (PROP(I,5)) = 0.3000E+00
 AIR ENTRY PRESSURE HEAD..... (PROP(I,6)) = 0.0000E+00

IRREDUCIBLE NAPL SATURATIONSNIRWN(I)= 0.1000E+00
 CRITICAL 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 = 0.1000E-08

FLUID PHASE NUMBER: 2

REFERENCE DENSITY..... = 0.9500E+03
 REFERENCE DYNAMIC VISCOSITY..... = 0.1000E-02
 COMPRESSIBILITY = 0.1000E-08

FLUID RETENTION DATA FOR SOIL MATERIAL NO. 1
 =====

IRREDUCIBLE WETTING-PHASE SATURATIONPROP(I,7)= 0.2000E+00
 NAPL REL. PERM. AT SWr.....AKSTAR(I)= 0.6800E+00
 N-W CAPILLARY PRESSURE @ Sw=1.....PCNSW1(I)= 0.0000E+00

TABULATED REL. PERM. AND CAP. PRESSURE DATA FOR SOIL MATERIAL NO. 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 NO. 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 SPECIFICATION DATA

NUMBER OF ROWS.....(NROWS) = 21
 NUMBER OF COLUMNS.....(NCOLS) = 2
 MAXIMUM ALLOWABLE X-SPACING.....(DXMAX) = 1.00
 MAXIMUM ALLOWABLE Y-SPACING.....(DYMAX) = 0.25
 INPUT INDICATOR FOR GRIDLINE COORD.....(IXYZRD) = 0
 HORIZONTAL PLANE DOMAIN INDICATOR.....(IHORGR) = 0

 X-INCREMENT OF THE FIRST GRID BLOCK(DX) = 1.000
 Y-INCREMENT OF THE FIRST GRID BLOCK(DY) = 0.250
 MAXIMUM VALUE OF X-COORDINATE(X0) = 1.000
 MAXIMUM VALUE OF Y-COORDINATE(Y0) = 5.000
 X-INCREMENT MULTIPLIER(SCFX) = 1.000
 Y-INCREMENT MULTIPLIER(SCFY) = 1.000
 MINIMUM VALUE OF X-COORDINATE(XSTART) = 0.000
 MINIMUM VALUE OF Y-COORDINATE(YSTART) = 0.000

*** FINITE-ELEMENT MESH NODAL CONNECTIONS ***

(NUMBERING IS COUNTER-CLOCKWISE)

ELEMENT	ELEMENTAL NODE NUMBERING				ELEMENT	ELEMENTAL NODE NUMBERING			
1	1	2	4	3	2	3	4	6	5
3	5	6	8	7	4	7	8	10	9
5	9	10	12	11	6	11	12	14	13
7	13	14	16	15	8	15	16	18	17
9	17	18	20	19	10	19	20	22	21
11	21	22	24	23	12	23	24	26	25
13	25	26	28	27	14	27	28	30	29
15	29	30	32	31	16	31	32	34	33
17	33	34	36	35	18	35	36	38	37
19	37	38	40	39	20	39	40	42	41

*** NODAL COORDINATES ***

NODE	X-COOR.	Y-COOR.	NODE	X-COOR.	Y-COOR.
1	0.00	0.00	2	1.00	0.00
3	0.00	0.25	4	1.00	0.25
5	0.00	0.50	6	1.00	0.50
7	0.00	0.75	8	1.00	0.75
9	0.00	1.00	10	1.00	1.00
11	0.00	1.25	12	1.00	1.25
13	0.00	1.50	14	1.00	1.50
15	0.00	1.75	16	1.00	1.75
17	0.00	2.00	18	1.00	2.00
19	0.00	2.25	20	1.00	2.25
21	0.00	2.50	22	1.00	2.50
23	0.00	2.75	24	1.00	2.75
25	0.00	3.00	26	1.00	3.00
27	0.00	3.25	28	1.00	3.25
29	0.00	3.50	30	1.00	3.50
31	0.00	3.75	32	1.00	3.75
33	0.00	4.00	34	1.00	4.00
35	0.00	4.25	36	1.00	4.25
37	0.00	4.50	38	1.00	4.50
39	0.00	4.75	40	1.00	4.75
41	0.00	5.00	42	1.00	5.00

BOUNDARY CONDITION DATA

NUMBER OF STEADY DIRICHLET BOUNDARIES (NBTO) = 4
 NUMBER OF STEADY FLUX BOUNDARIES (NDFLUX) = 4
 NUMBER OF TRANSIENT DIRICHLET BOUNDARIES.... (NBHVAR) = 0
 NUMBER OF TRANSIENT FLUX BOUNDARIES..... (NBFVAR) = 0

STEADY-STATE DIRICHLET BOUNDARY CONDITIONS

INDEX	NODE NO.	D.V. NO.	PRESCRIBED VALUE	B.C. IDENTIFIER
1	1	1	150000.	-1
2	1	2	150000.	-1

3	2	1	150000.	-1
4	2	2	150000.	-1

STEADY-STATE FLUX BOUNDARY CONDITIONS

INDEX	NODE NO.	D.V. NO.	FLUID FLUX VALUE
1	41	1	1.585000E-06
2	41	2	1.426900E-05
3	42	1	1.585000E-06
4	42	2	1.426900E-05

 * INITIAL CONDITION FOR FLOW PROBLEM *

NODE	PRES. (PH.1)	SAT. (PH. 1)	SAT. (PH. 2)	PRES. (PH. 2)	SAT. (PH. 3)	PRES. (PH.3)
1	0.134323E+06	0.1000E+01	0.0000E+00	0.134323E+06	0.0000E+00	0.100000E+06
3	0.131871E+06	0.1000E+01	0.0000E+00	0.131871E+06	0.0000E+00	0.100000E+06
5	0.129420E+06	0.1000E+01	0.0000E+00	0.129420E+06	0.0000E+00	0.100000E+06
7	0.126968E+06	0.1000E+01	0.0000E+00	0.126968E+06	0.0000E+00	0.100000E+06
9	0.124516E+06	0.1000E+01	0.0000E+00	0.124516E+06	0.0000E+00	0.100000E+06
11	0.122065E+06	0.1000E+01	0.0000E+00	0.122065E+06	0.0000E+00	0.100000E+06
13	0.119613E+06	0.1000E+01	0.0000E+00	0.119613E+06	0.0000E+00	0.100000E+06
15	0.117162E+06	0.1000E+01	0.0000E+00	0.117162E+06	0.0000E+00	0.100000E+06
17	0.114710E+06	0.1000E+01	0.0000E+00	0.114710E+06	0.0000E+00	0.100000E+06
19	0.112258E+06	0.1000E+01	0.0000E+00	0.112258E+06	0.0000E+00	0.100000E+06
21	0.109807E+06	0.1000E+01	0.0000E+00	0.109807E+06	0.0000E+00	0.100000E+06
23	0.107355E+06	0.1000E+01	0.0000E+00	0.107355E+06	0.0000E+00	0.100000E+06
25	0.104903E+06	0.1000E+01	0.0000E+00	0.104903E+06	0.0000E+00	0.100000E+06
27	0.102452E+06	0.1000E+01	0.0000E+00	0.102452E+06	0.0000E+00	0.100000E+06
29	0.100000E+06	0.1000E+01	0.0000E+00	0.100000E+06	0.0000E+00	0.100000E+06
31	0.997273E+05	0.9727E+00	0.0000E+00	0.997273E+05	0.2727E-01	0.100000E+06
33	0.994545E+05	0.9455E+00	0.0000E+00	0.994545E+05	0.5455E-01	0.100000E+06
35	0.991818E+05	0.9182E+00	0.0000E+00	0.991818E+05	0.8182E-01	0.100000E+06
37	0.989091E+05	0.8909E+00	0.0000E+00	0.989091E+05	0.1091E+00	0.100000E+06
39	0.986364E+05	0.8636E+00	0.0000E+00	0.986364E+05	0.1364E+00	0.100000E+06
41	0.983636E+05	0.8364E+00	0.0000E+00	0.983636E+05	0.1636E+00	0.100000E+06
2	0.134323E+06	0.1000E+01	0.0000E+00	0.134323E+06	0.0000E+00	0.100000E+06
4	0.131871E+06	0.1000E+01	0.0000E+00	0.131871E+06	0.0000E+00	0.100000E+06
6	0.129420E+06	0.1000E+01	0.0000E+00	0.129420E+06	0.0000E+00	0.100000E+06
8	0.126968E+06	0.1000E+01	0.0000E+00	0.126968E+06	0.0000E+00	0.100000E+06
10	0.124516E+06	0.1000E+01	0.0000E+00	0.124516E+06	0.0000E+00	0.100000E+06
12	0.122065E+06	0.1000E+01	0.0000E+00	0.122065E+06	0.0000E+00	0.100000E+06
14	0.119613E+06	0.1000E+01	0.0000E+00	0.119613E+06	0.0000E+00	0.100000E+06
16	0.117162E+06	0.1000E+01	0.0000E+00	0.117162E+06	0.0000E+00	0.100000E+06
18	0.114710E+06	0.1000E+01	0.0000E+00	0.114710E+06	0.0000E+00	0.100000E+06
20	0.112258E+06	0.1000E+01	0.0000E+00	0.112258E+06	0.0000E+00	0.100000E+06
22	0.109807E+06	0.1000E+01	0.0000E+00	0.109807E+06	0.0000E+00	0.100000E+06
24	0.107355E+06	0.1000E+01	0.0000E+00	0.107355E+06	0.0000E+00	0.100000E+06
26	0.104903E+06	0.1000E+01	0.0000E+00	0.104903E+06	0.0000E+00	0.100000E+06
28	0.102452E+06	0.1000E+01	0.0000E+00	0.102452E+06	0.0000E+00	0.100000E+06
30	0.100000E+06	0.1000E+01	0.0000E+00	0.100000E+06	0.0000E+00	0.100000E+06
32	0.997273E+05	0.9727E+00	0.0000E+00	0.997273E+05	0.2727E-01	0.100000E+06
34	0.994545E+05	0.9455E+00	0.0000E+00	0.994545E+05	0.5455E-01	0.100000E+06
36	0.991818E+05	0.9182E+00	0.0000E+00	0.991818E+05	0.8182E-01	0.100000E+06
38	0.989091E+05	0.8909E+00	0.0000E+00	0.989091E+05	0.1091E+00	0.100000E+06
40	0.986364E+05	0.8636E+00	0.0000E+00	0.986364E+05	0.1364E+00	0.100000E+06
42	0.983636E+05	0.8364E+00	0.0000E+00	0.983636E+05	0.1636E+00	0.100000E+06

LIST OF BOUNDARY NODE NUMBERS

1 2 41 42

DISTANCE SCALE FACTOR FOR PRESSURE B.C.INCORPORATION = 0.40000E+01

MATRIX BANDWIDTH REQUIRED FOR FLOW SIMULATION = 15
 =====

+++++++ BEGIN TRANSIENT CALCULATIONS ++++++

 *** ELAPSED TIME: 1000. TIME STEP: 1 TIME STEP SIZE: 0.100E+04 ***

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM HEAD ERROR	NODE NUMBER	MAXIMUM SATUR. ERROR	NODE NUMBER	RELAXATION FACTOR
1	40	0.3356	29	0.997E-03	41	1.00
2	34	0.1521	31	0.447E-02	36	1.00
3	0	-0.8792E-02	31	0.477E-02	41	0.962

 *** ELAPSED TIME: 2082. TIME STEP: 2 TIME STEP SIZE: 0.108E+04 ***

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM HEAD ERROR	NODE NUMBER	MAXIMUM SATUR. ERROR	NODE NUMBER	RELAXATION FACTOR
1	42	0.1227	1	0.172E-02	42	1.00
2	38	0.1765	33	0.133E-01	38	1.00
3	36	0.1360E-01	37	0.573E-02	41	1.00
4	2	-0.2597E-02	41	0.136E-01	41	0.880
5	2	-0.2597E-02	41	0.206E-01	41	1.00
6	0	0.8508E-02	41	0.849E-02	40	0.153

 *** ELAPSED TIME: 3538. TIME STEP: 3 TIME STEP SIZE: 0.146E+04 ***

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM HEAD ERROR	NODE NUMBER	MAXIMUM SATUR. ERROR	NODE NUMBER	RELAXATION FACTOR
1	42	0.6565E-01	1	0.165E-01	41	1.00
2	38	0.1024	35	0.458E-02	37	1.00

3 0 0.6066E-02 39 0.582E-02 40 1.00

*** ELAPSED TIME: 6703. TIME STEP: 4 TIME STEP SIZE: 0.316E+04 ***

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM HEAD ERROR	NODE NUMBER	MAXIMUM SATUR. ERROR	NODE NUMBER	RELAXATION FACTOR
1	44	0.8239E-01	1	0.418E-01	41	1.00
2	0	-0.3199E-02	41	0.404E-06	41	0.974

*** ELAPSED TIME: 0.1106E+05 TIME STEP: 5 TIME STEP SIZE: 0.436E+04 ***

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM HEAD ERROR	NODE NUMBER	MAXIMUM SATUR. ERROR	NODE NUMBER	RELAXATION FACTOR
1	42	-0.3793E-01	41	0.533E-01	41	1.00
2	0	-0.5848E-02	39	0.650E-02	40	1.00

*** ELAPSED TIME: 0.1697E+05 TIME STEP: 6 TIME STEP SIZE: 0.590E+04 ***

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM HEAD ERROR	NODE NUMBER	MAXIMUM SATUR. ERROR	NODE NUMBER	RELAXATION FACTOR
1	4	-0.3798E-01	41	0.587E-01	41	1.00
2	0	0.9684E-02	1	0.637E-02	37	0.843

*** ELAPSED TIME: 0.2659E+05 TIME STEP: 7 TIME STEP SIZE: 0.962E+04 ***

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM HEAD ERROR	NODE NUMBER	MAXIMUM SATUR. ERROR	NODE NUMBER	RELAXATION FACTOR
1	4	-0.3702E-01	41	0.502E-01	42	1.00
2	0	0.9534E-02	41	0.703E-02	39	0.842

*** ELAPSED TIME: 0.6069E+05 TIME STEP: 8 TIME STEP SIZE: 0.341E+05 ***

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM HEAD ERROR	NODE NUMBER	MAXIMUM SATUR. ERROR	NODE NUMBER	RELAXATION FACTOR
1	46	-0.3455E-01	41	0.843E-01	41	1.00
2	42	0.5428E-01	41	0.340E-05	39	0.318
3	42	0.3615E-01	41	0.234E-05	39	1.00
4	0	0.7203E-02	41	0.322E-06	41	1.00

 *** ELAPSED TIME: 0.2312E+06 TIME STEP: 9 TIME STEP SIZE: 0.171E+06 ***

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM HEAD ERROR	NODE NUMBER	MAXIMUM SATUR. ERROR	NODE NUMBER	RELAXATION FACTOR
1	46	-0.7259E-01	41	0.221	42	0.903
2	44	0.4015E-01	41	0.132E-01	41	0.661
3	2	0.1225E-01	41	0.449E-02	41	1.00
4	40	0.1023E-01	37	0.973E-02	37	1.00
5	40	-0.1063E-01	37	0.532E-03	41	0.481
6	40	-0.1063E-01	37	0.498E-02	39	1.00
7	0	0.5829E-02	37	0.190E-02	42	0.691

 *** ELAPSED TIME: 0.3846E+06 TIME STEP: 10 TIME STEP SIZE: 0.153E+06 ***

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM HEAD ERROR	NODE NUMBER	MAXIMUM SATUR. ERROR	NODE NUMBER	RELAXATION FACTOR
1	46	0.1465E-01	41	0.123	41	1.00
2	50	0.3991E-01	37	0.643E-01	41	1.00
3	50	-0.7137E-01	39	0.305E-01	41	0.280
4	44	-0.5217E-01	39	0.193E-01	41	1.00
5	0	0.9558E-02	41	0.727E-03	39	0.885

*** NODAL FLUID FLUX VALUES ***

NODAL FLUXES FOR FLUID PHASE # 1

NODE	FLUID FLUX	NODE	FLUID FLUX	NODE	FLUID FLUX	NODE	FLUID FLUX	NODE	FLUID FLUX
1	0.0000E+00	2	0.0000E+00	41	1.5850E-06	42	1.5850E-06		

.....
 SUM OF ABOVE FLUX VALUES = 3.17000E-06

NODAL FLUXES FOR FLUID PHASE # 2

NODE	FLUID FLUX	NODE	FLUID FLUX	NODE	FLUID FLUX	NODE	FLUID FLUX	NODE	FLUID FLUX
1	0.0000E+00	2	0.0000E+00	41	1.4269E-05	42	1.4269E-05		

SUM OF ABOVE FLUX VALUES = 2.85380E-05

*** NODAL PRESSURE VALUES ***

NODE	PRESSURE (Pw)	NODE	PRESSURE (Pw)	NODE	PRESSURE (Pw)	NODE	PRESSURE (Pw)	NODE	PRESSURE (Pw)
1	1.43992E+05	2	1.43992E+05	3	1.41541E+05	4	1.41541E+05	5	1.39089E+05
6	1.39089E+05	7	1.36637E+05	8	1.36637E+05	9	1.34186E+05	10	1.34186E+05
11	1.31734E+05	12	1.31734E+05	13	1.29282E+05	14	1.29282E+05	15	1.26831E+05
16	1.26831E+05	17	1.24379E+05	18	1.24379E+05	19	1.21928E+05	20	1.21928E+05
21	1.19476E+05	22	1.19476E+05	23	1.17024E+05	24	1.17024E+05	25	1.14573E+05
26	1.14573E+05	27	1.12121E+05	28	1.12121E+05	29	1.09669E+05	30	1.09669E+05
31	1.07218E+05	32	1.07218E+05	33	1.04766E+05	34	1.04766E+05	35	1.02314E+05
36	1.02314E+05	37	99863.	38	99863.	39	97409.	40	97409.
41	94971.	42	94971.						

*** NODAL VALUES OF NAPL SATURATION ***

NODE	SATURAT. (Sn)	NODE	SATURAT. (Sn)	NODE	SATURAT. (Sn)	NODE	SATURAT. (Sn)	NODE	SATURAT. (Sn)
1	0.00000E+00	2	0.00000E+00	3	0.00000E+00	4	0.00000E+00	5	0.00000E+00
6	0.00000E+00	7	0.00000E+00	8	0.00000E+00	9	0.00000E+00	10	0.00000E+00
11	0.00000E+00	12	0.00000E+00	13	0.00000E+00	14	0.00000E+00	15	0.00000E+00
16	0.00000E+00	17	0.00000E+00	18	0.00000E+00	19	0.00000E+00	20	0.00000E+00
21	0.00000E+00	22	0.00000E+00	23	0.00000E+00	24	0.00000E+00	25	0.00000E+00
26	0.00000E+00	27	0.00000E+00	28	0.00000E+00	29	0.00000E+00	30	0.00000E+00
31	0.00000E+00	32	0.00000E+00	33	0.00000E+00	34	0.00000E+00	35	0.00000E+00
36	0.00000E+00	37	0.00000E+00	38	0.00000E+00	39	4.58236E-02	40	4.58236E-02
41	0.21645	42	0.21645						

*** NODAL VALUES OF WATER SATURATION ***

NODE	SATURAT. (Sw)	NODE	SATURAT. (Sw)	NODE	SATURAT. (Sw)	NODE	SATURAT. (Sw)	NODE	SATURAT. (Sw)
1	1.0000	2	1.0000	3	1.0000	4	1.0000	5	1.0000
6	1.0000	7	1.0000	8	1.0000	9	1.0000	10	1.0000
11	1.0000	12	1.0000	13	1.0000	14	1.0000	15	1.0000
16	1.0000	17	1.0000	18	1.0000	19	1.0000	20	1.0000
21	1.0000	22	1.0000	23	1.0000	24	1.0000	25	1.0000
26	1.0000	27	1.0000	28	1.0000	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	0.98627	38	0.98627	39	0.77881	40	0.77881
41	0.46902	42	0.46902						

*** FLUID FLOW MASS BALANCE INFORMATION AT TIME = 0.3846E+06***

*** MASS BALANCE, FLUID, AND FLOW INFORMATION ***

FLUID PHASE NUMBER 1
 NET FLOW RATE DUE TO BOUNDARY FLUX AND SINKS 3.17000E-06
 RATE OF FLUID ACCUMULATION 1.85000E-06
 MASS BALANCE ERROR 1.32000E-06
 NORMALIZED MASS BALANCE ERROR 2.62948E-01
 CUMULATIVE FLUID STORAGE -7.12909E-01

*** MASS BALANCE, FLUID, AND FLOW INFORMATION ***

FLUID PHASE NUMBER 2
 NET FLOW RATE DUE TO BOUNDARY FLUX AND SINKS 2.85380E-05
 RATE OF FLUID ACCUMULATION 2.85380E-05
 MASS BALANCE ERROR 3.26301E-14
 NORMALIZED MASS BALANCE ERROR 5.71696E-10
 CUMULATIVE FLUID STORAGE 1.09761E+01

 *** ELAPSED TIME: 0.8002E+06 TIME STEP: 11 TIME STEP SIZE: 0.416E+06 ***

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM HEAD ERROR	NODE NUMBER	MAXIMUM SATUR. ERROR	NODE NUMBER	RELAXATION FACTOR
1	44	-0.8703E-01	39	0.164	39	1.00
2	50	0.7374E-01	39	0.547E-01	37	0.560
3	48	0.4492E-01	37	0.300E-01	39	1.00
4	0	0.5016E-02	41	0.415E-02	37	1.00

 *** ELAPSED TIME: 0.1563E+07 TIME STEP: 12 TIME STEP SIZE: 0.762E+06 ***

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM HEAD ERROR	NODE NUMBER	MAXIMUM SATUR. ERROR	NODE NUMBER	RELAXATION FACTOR
1	50	-0.2419E-01	37	0.289	37	0.693
2	50	0.9898E-01	35	0.140	35	0.846E-01
3	54	0.9590E-01	33	0.931E-01	35	1.00
4	54	0.1411	35	0.164	39	1.00
5	16	0.3305E-02	41	0.564E-01	33	1.00
6	8	0.9260E-03	31	0.276E-01	39	1.00
7	0	-0.3649E-02	41	0.388E-02	35	0.127

 *** ELAPSED TIME: 0.2217E+07 TIME STEP: 13 TIME STEP SIZE: 0.654E+06 ***

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM HEAD ERROR	NODE NUMBER	MAXIMUM SATUR. ERROR	NODE NUMBER	RELAXATION FACTOR
1	58	0.2005	41	0.260	40	0.768
2	62	0.8640	39	0.881	41	0.227
3	54	0.1792E+07	41	0.114	39	1.00
4	58	-0.1792E+07	1	0.143	33	0.500
5	62	-0.8960E+06	1	0.973E-01	31	1.00
6	20	0.3535E-03	41	0.189E-01	31	1.000
7	0	0.3010E-03	33	0.756E-02	41	1.00

 *** ELAPSED TIME: 0.2634E+07 TIME STEP: 14 TIME STEP SIZE: 0.417E+06 ***

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM HEAD ERROR	NODE NUMBER	MAXIMUM SATUR. ERROR	NODE NUMBER	RELAXATION FACTOR
1	30	-0.1058E-01	41	0.807E-01	31	1.00
2	12	-0.7270E-02	29	0.866E-01	29	1.00
3	14	0.9177E-02	29	0.278E-01	29	0.396
4	10	0.7914E-02	27	0.297E-01	33	1.00
5	18	0.8295E-02	15	0.523E-01	29	1.00
6	18	-0.9917E-02	23	0.382E-01	29	0.418
7	10	0.9195E-02	11	0.284E-01	29	0.226
8	6	0.9181E-02	11	0.375E-01	29	1.00
9	2	0.8081E-02	27	0.109E-01	37	1.00
10	22	0.9562E-02	7	0.616E-01	29	1.00

..... SOLUTION NOT CONVERGING.....
 WORST HEAD ERROR = 0.9562E-02
 WORST SATURATION ERROR = 0.6163E-01

COMPUTATIONAL TIME STEP VALUE = 0.4169E+05 CURRENT TIME = 0.2259E+07

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM HEAD ERROR	NODE NUMBER	MAXIMUM SATUR. ERROR	NODE NUMBER	RELAXATION FACTOR
1	6	-0.1131E-01	41	0.665E-02	33	1.00
2	26	-0.2093E-01	35	0.861E-02	33	1.00
3	26	0.2128E-01	35	0.167E-02	33	0.492
4	22	0.1835E-01	31	0.103E-02	31	1.00
5	4	0.1165E-01	35	0.947E-03	33	1.00
6	6	-0.1102E-01	35	0.453E-03	31	0.520
7	6	-0.1090E-01	35	0.424E-03	33	1.00
8	0	0.9727E-02	23	0.169E-03	31	0.541

COMPUTATIONAL TIME STEP VALUE = 0.2085E+06 CURRENT TIME = 0.2467E+07

NUMBER OF NON-CONVERGENT MAXIMUM HEAD NODE MAXIMUM SATUR. NODE RELAXATION

ITERATION	NODES	ERROR	NUMBER	ERROR	NUMBER	FACTOR
1	16	0.7308E-02	5	0.270E-01	31	1.00
2	12	0.7037E-02	5	0.159E-01	41	1.00
3	0	0.7551E-02	5	0.463E-02	29	1.00

COMPUTATIONAL TIME STEP VALUE = 0.1668E+06 CURRENT TIME = 0.2634E+07

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM HEAD ERROR	NODE NUMBER	MAXIMUM SATUR. ERROR	NODE NUMBER	RELAXATION FACTOR
1	10	-0.1459E-01	5	0.286E-01	29	1.00
2	6	-0.8362E-02	17	0.142E-01	33	1.00
3	4	0.7356E-02	17	0.144E-01	35	0.547
4	6	0.1235E-01	41	0.871E-02	31	1.00
5	2	0.8301E-02	35	0.119E-01	31	1.00
6	0	-0.9803E-02	35	0.806E-02	31	0.423

 *** ELAPSED TIME: 0.3468E+07 TIME STEP: 15 TIME STEP SIZE: 0.834E+06 ***

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM HEAD ERROR	NODE NUMBER	MAXIMUM SATUR. ERROR	NODE NUMBER	RELAXATION FACTOR
1	32	0.1642E-01	19	0.194	29	1.00
2	18	0.1309E-01	13	0.122	27	1.00
3	26	-0.1299E-01	13	0.340E-01	25	0.503
4	22	-0.1291E-01	13	0.248E-01	25	1.00
5	18	-0.7293E-02	9	0.419E-01	25	1.00
6	10	-0.1418E-01	23	0.161E-01	35	1.00
7	14	0.7163E-02	9	0.229E-01	35	0.712
8	2	0.7752E-02	15	0.122E-01	31	1.00
9	2	0.7703E-02	15	0.144E-01	35	1.00
10	8	-0.1413E-01	11	0.162E-01	33	0.272

..... SOLUTION NOT CONVERGING.....
 WORST HEAD ERROR = -0.1413E-01
 WORST SATURATION ERROR = 0.1622E-01

COMPUTATIONAL TIME STEP VALUE = 0.8339E+05 CURRENT TIME = 0.2717E+07

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM HEAD ERROR	NODE NUMBER	MAXIMUM SATUR. ERROR	NODE NUMBER	RELAXATION FACTOR
1	6	0.1642E-01	19	0.178E-01	29	1.00
2	6	-0.1325E-01	35	0.802E-02	39	0.576
3	0	-0.8531E-02	7	0.956E-02	39	1.00

COMPUTATIONAL TIME STEP VALUE = 0.4169E+06 CURRENT TIME = 0.3134E+07

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM HEAD ERROR	NODE NUMBER	MAXIMUM SATUR. ERROR	NODE NUMBER	RELAXATION FACTOR
1	28	0.9848E-02	41	0.866E-01	29	1.00
2	16	0.6185E-02	23	0.545E-01	27	1.00

3	16	0.7634E-02	23	0.357E-01	31	1.00
4	12	-0.1383E-01	23	0.193E-01	27	0.276
5	10	-0.1352E-01	23	0.139E-01	27	1.00
6	4	-0.1476E-01	25	0.127E-01	29	1.00
7	8	-0.1111E-01	19	0.157E-01	27	1.00
8	6	0.1022E-01	13	0.138E-01	41	0.531
9	8	-0.6281E-02	7	0.251E-01	27	0.432
10	2	-0.6352E-02	37	0.116E-01	27	1.00

..... SOLUTION NOT CONVERGING.....
 WORST HEAD ERROR = -0.6352E-02
 WORST SATURATION ERROR = 0.1159E-01

COMPUTATIONAL TIME STEP VALUE = 0.4169E+05 CURRENT TIME = 0.2759E+07

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM HEAD ERROR	NODE NUMBER	MAXIMUM SATUR. ERROR	NODE NUMBER	RELAXATION FACTOR
1	2	0.1028E-01	41	0.711E-02	29	1.00
2	4	-0.1068E-01	9	0.766E-02	29	0.481
3	2	-0.1053E-01	9	0.722E-02	29	1.00
4	0	-0.7792E-02	35	0.715E-02	29	1.00

COMPUTATIONAL TIME STEP VALUE = 0.2085E+06 CURRENT TIME = 0.2968E+07

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM HEAD ERROR	NODE NUMBER	MAXIMUM SATUR. ERROR	NODE NUMBER	RELAXATION FACTOR
1	28	0.1915E-01	33	0.369E-01	29	1.00
2	12	0.1142E-01	11	0.192E-01	27	1.00
3	10	-0.1191E-01	11	0.148E-01	37	0.480
4	8	-0.1192E-01	11	0.192E-01	27	1.00
5	0	-0.5930E-02	17	0.985E-02	33	1.00

COMPUTATIONAL TIME STEP VALUE = 0.5003E+06 CURRENT TIME = 0.3468E+07

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM HEAD ERROR	NODE NUMBER	MAXIMUM SATUR. ERROR	NODE NUMBER	RELAXATION FACTOR
1	28	0.9111E-02	17	0.446E-01	37	1.00
2	20	0.9062E-02	17	0.812E-01	27	1.00
3	0	-0.8513E-02	17	0.879E-02	41	0.523

 *** ELAPSED TIME: 0.4332E+07 TIME STEP: 16 TIME STEP SIZE: 0.864E+06 ***

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM HEAD ERROR	NODE NUMBER	MAXIMUM SATUR. ERROR	NODE NUMBER	RELAXATION FACTOR
1	32	-0.7384E-02	9	0.117	27	1.00
2	36	-0.7366E-02	9	0.199	25	1.00
3	12	-0.7366E-02	9	0.801E-01	23	1.00
4	26	0.1451E-01	9	0.329E-01	25	0.254
5	28	0.1462E-01	9	0.308E-01	25	1.00
6	40	0.1359E-01	19	0.889E-01	25	1.00
7	32	0.6118E-02	7	0.994E-01	25	1.00
8	22	0.6134E-02	7	0.994E-01	25	1.00

9	22	0.7851E-02	15	0.932E-01	25	1.00
10	10	0.1790E-01	21	0.179E-01	33	1.00

..... SOLUTION NOT CONVERGING.....
 WORST HEAD ERROR = 0.1790E-01
 WORST SATURATION ERROR = 0.1786E-01

COMPUTATIONAL TIME STEP VALUE = 0.8640E+05 CURRENT TIME = 0.3554E+07

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM HEAD ERROR	NODE NUMBER	MAXIMUM SATUR. ERROR	NODE NUMBER	RELAXATION FACTOR
1	4	0.8605E-02	15	0.116E-01	27	1.00
2	4	-0.1320E-01	15	0.738E-02	41	0.326
3	4	-0.1312E-01	15	0.767E-02	41	1.00
4	4	0.1091E-01	25	0.855E-02	29	0.566
5	20	0.1477E-01	25	0.687E-02	33	1.00
6	0	-0.6438E-02	25	0.577E-02	33	0.746

COMPUTATIONAL TIME STEP VALUE = 0.4320E+06 CURRENT TIME = 0.3986E+07

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM HEAD ERROR	NODE NUMBER	MAXIMUM SATUR. ERROR	NODE NUMBER	RELAXATION FACTOR
1	32	0.7009E-02	11	0.356E-01	27	1.00
2	8	0.7073E-02	11	0.393E-01	25	1.00
3	2	-0.6539E-02	11	0.106E-01	35	0.529
4	2	-0.6840E-02	11	0.132E-01	35	1.00
5	4	0.1342E-01	9	0.915E-02	29	0.255
6	6	0.1341E-01	9	0.103E-01	29	1.00
7	0	0.6346E-02	15	0.831E-02	33	1.00

COMPUTATIONAL TIME STEP VALUE = 0.3456E+06 CURRENT TIME = 0.4332E+07

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM HEAD ERROR	NODE NUMBER	MAXIMUM SATUR. ERROR	NODE NUMBER	RELAXATION FACTOR
1	28	-0.1521E-01	7	0.548E-01	25	1.00
2	16	-0.9911E-02	23	0.548E-01	25	1.00
3	14	0.8822E-02	21	0.247E-01	25	0.542
4	12	0.1075E-01	23	0.256E-01	25	1.00
5	2	0.1397E-01	11	0.983E-02	29	1.00
6	2	0.1584E-01	5	0.786E-02	31	1.00
7	2	0.9118E-02	19	0.102E-01	31	1.00
8	4	0.1175E-01	31	0.520E-02	31	1.00
9	0	0.9550E-02	13	0.360E-02	25	1.00

 *** ELAPSED TIME: 0.5196E+07 TIME STEP: 17 TIME STEP SIZE: 0.864E+06 ***

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM HEAD ERROR	NODE NUMBER	MAXIMUM SATUR. ERROR	NODE NUMBER	RELAXATION FACTOR
1	36	-0.9768E-02	13	0.767E-01	25	1.00
2	20	-0.9776E-02	13	0.132	23	1.00
3	30	0.1024E-01	13	0.282E-01	23	0.477
4	22	0.9884E-02	13	0.355E-01	21	1.00
5	0	0.5233E-02	9	0.992E-02	25	1.00

 *** ELAPSED TIME: 0.6060E+07 TIME STEP: 18 TIME STEP SIZE: 0.864E+06 ***

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM HEAD ERROR	NODE NUMBER	MAXIMUM SATUR. ERROR	NODE NUMBER	RELAXATION FACTOR
1	42	-0.1752E-01	9	0.107	21	1.00
2	6	-0.1017E-01	17	0.203E-01	27	1.00
3	8	0.1036E-01	17	0.142E-01	23	0.491
4	6	0.1035E-01	17	0.170E-01	23	1.00
5	0	-0.4994E-02	17	0.976E-02	23	0.723

 *** ELAPSED TIME: 0.6924E+07 TIME STEP: 19 TIME STEP SIZE: 0.864E+06 ***

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM HEAD ERROR	NODE NUMBER	MAXIMUM SATUR. ERROR	NODE NUMBER	RELAXATION FACTOR
1	48	0.1514E-01	3	0.107	21	1.00
2	16	0.9070E-02	7	0.137	19	1.00
3	16	0.9438E-02	7	0.315E-01	19	1.00
4	14	-0.1830E-01	7	0.630E-01	17	0.258
5	12	-0.1849E-01	7	0.479E-01	17	1.00
6	6	0.1292E-01	5	0.155E-01	25	0.622
7	24	0.1293E-01	5	0.768E-01	17	1.00
8	14	-0.7999E-02	5	0.740E-01	19	0.658
9	8	-0.8066E-02	5	0.202E-01	19	1.00
10	2	-0.5867E-02	7	0.123E-01	25	1.00

..... SOLUTION NOT CONVERGING.....
 WORST HEAD ERROR = -0.5867E-02
 WORST SATURATION ERROR = 0.1229E-01

COMPUTATIONAL TIME STEP VALUE = 0.8640E+05 CURRENT TIME = 0.6146E+07

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM HEAD ERROR	NODE NUMBER	MAXIMUM SATUR. ERROR	NODE NUMBER	RELAXATION FACTOR
1	8	0.1514E-01	3	0.103E-01	21	1.00
2	8	-0.1079E-01	5	0.119E-01	39	0.616
3	4	-0.1006E-01	5	0.117E-01	41	1.00
4	2	0.8944E-02	41	0.109E-01	25	0.543
5	16	0.1401E-01	41	0.536E-02	37	1.00
6	0	-0.7405E-02	41	0.405E-02	39	0.700

COMPUTATIONAL TIME STEP VALUE = 0.4320E+06 CURRENT TIME = 0.6578E+07

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM HEAD ERROR	NODE NUMBER	MAXIMUM SATUR. ERROR	NODE NUMBER	RELAXATION FACTOR
1	32	0.6146E-02	15	0.520E-01	21	1.00
2	14	0.5372E-02	15	0.249E-01	21	1.00
3	4	0.5060E-02	19	0.140E-01	19	1.00
4	2	-0.5429E-02	15	0.113E-01	23	0.466
5	2	0.6083E-02	13	0.142E-01	23	0.208
6	2	0.6087E-02	13	0.154E-01	23	1.00
7	2	-0.1081E-01	9	0.844E-02	31	0.281
8	4	-0.1081E-01	9	0.846E-02	31	1.00

9	2	-0.8984E-02	13	0.141E-01	21	1.00
10	2	0.9717E-02	29	0.107E-01	31	0.462

..... SOLUTION NOT CONVERGING.....
 WORST HEAD ERROR = 0.9717E-02
 WORST SATURATION ERROR = 0.1072E-01

COMPUTATIONAL TIME STEP VALUE = 0.4320E+05 CURRENT TIME = 0.6190E+07

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM HEAD ERROR	NODE NUMBER	MAXIMUM SATUR. ERROR	NODE NUMBER	RELAXATION FACTOR
1	6	0.1217E-01	21	0.855E-02	25	1.00
2	16	-0.1191E-01	41	0.593E-02	19	0.508
3	14	-0.1192E-01	41	0.593E-02	19	1.00
4	0	0.9505E-02	15	0.618E-02	25	0.580

COMPUTATIONAL TIME STEP VALUE = 0.2160E+06 CURRENT TIME = 0.6406E+07

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM HEAD ERROR	NODE NUMBER	MAXIMUM SATUR. ERROR	NODE NUMBER	RELAXATION FACTOR
1	4	0.9016E-02	31	0.219E-01	21	1.00
2	10	-0.9398E-02	9	0.157E-01	19	0.480
3	6	-0.7118E-02	41	0.135E-01	39	1.00
4	4	0.1389E-01	41	0.145E-01	23	0.256
5	4	0.1396E-01	41	0.154E-01	23	1.00
6	4	0.7754E-02	39	0.108E-01	23	1.00
7	2	-0.1020E-01	39	0.670E-02	33	0.380
8	2	-0.1017E-01	39	0.741E-02	27	1.00
9	0	-0.8009E-02	21	0.876E-02	33	1.00

COMPUTATIONAL TIME STEP VALUE = 0.5184E+06 CURRENT TIME = 0.6924E+07

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM HEAD ERROR	NODE NUMBER	MAXIMUM SATUR. ERROR	NODE NUMBER	RELAXATION FACTOR
1	44	0.8670E-02	17	0.314E-01	23	1.00
2	12	0.8705E-02	17	0.469E-01	19	1.00
3	0	0.9418E-02	17	0.746E-02	29	1.00

 *** ELAPSED TIME: 0.7788E+07 TIME STEP: 20 TIME STEP SIZE: 0.864E+06 ***

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM HEAD ERROR	NODE NUMBER	MAXIMUM SATUR. ERROR	NODE NUMBER	RELAXATION FACTOR
1	48	-0.1812E-01	17	0.125	19	1.00
2	22	0.1114E-01	13	0.117	17	0.660
3	12	0.1202E-01	13	0.276E-01	19	1.00
4	14	-0.1901E-01	13	0.199E-01	17	0.316
5	10	-0.1901E-01	13	0.249E-01	21	1.00
6	12	0.5576E-02	13	0.520E-01	17	0.822

7	6	0.5071E-02	13	0.167E-01	19	1.00
8	4	0.1242E-01	15	0.166E-01	17	1.00
9	6	-0.9800E-02	13	0.193E-01	17	0.584
10	8	-0.9961E-02	13	0.236E-01	17	1.00

..... SOLUTION NOT CONVERGING.....
 WORST HEAD ERROR = -0.9961E-02
 WORST SATURATION ERROR = 0.2361E-01

COMPUTATIONAL TIME STEP VALUE = 0.8640E+05 CURRENT TIME = 0.7010E+07

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM HEAD ERROR	NODE NUMBER	MAXIMUM SATUR. ERROR	NODE NUMBER	RELAXATION FACTOR
1	8	-0.1812E-01	17	0.897E-02	19	1.00
2	20	-0.1390E-01	41	0.104E-01	41	1.00
3	8	0.1156E-01	41	0.879E-02	19	0.566
4	22	0.1452E-01	41	0.573E-02	29	1.00
5	0	-0.7003E-02	41	0.558E-02	29	0.723

*** NODAL FLUID FLUX VALUES ***

NODAL FLUXES FOR FLUID PHASE # 1

NODE	FLUID FLUX	NODE	FLUID FLUX	NODE	FLUID FLUX	NODE	FLUID FLUX	NODE	FLUID FLUX
1	-1.6681E-05	2	-1.6681E-05	41	1.5850E-06	42	1.5850E-06		

SUM OF ABOVE FLUX VALUES = -3.01919E-05

NODAL FLUXES FOR FLUID PHASE # 2

NODE	FLUID FLUX	NODE	FLUID FLUX	NODE	FLUID FLUX	NODE	FLUID FLUX	NODE	FLUID FLUX
1	-0.0000E+00	2	-0.0000E+00	41	1.4269E-05	42	1.4269E-05		

SUM OF ABOVE FLUX VALUES = 2.85380E-05

COMPUTATIONAL TIME STEP VALUE = 0.4320E+06 CURRENT TIME = 0.7442E+07

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM HEAD ERROR	NODE NUMBER	MAXIMUM SATUR. ERROR	NODE NUMBER	RELAXATION FACTOR
1	32	0.7099E-02	17	0.529E-01	19	1.00
2	12	0.6040E-02	17	0.147E-01	25	1.00
3	2	0.7674E-02	17	0.129E-01	29	1.00

4	2	-0.1327E-01	17	0.662E-02	21	0.289
5	2	-0.1329E-01	17	0.749E-02	21	1.00
6	6	-0.1412E-01	11	0.105E-01	21	1.00
7	0	0.9171E-02	9	0.910E-02	25	0.644

*** NODAL FLUID FLUX VALUES ***

NODAL FLUXES FOR FLUID PHASE # 1

NODE	FLUID FLUX	NODE	FLUID FLUX	NODE	FLUID FLUX	NODE	FLUID FLUX	NODE	FLUID FLUX
1	-1.7673E-05	2	-1.7673E-05	41	1.5850E-06	42	1.5850E-06		

SUM OF ABOVE FLUX VALUES = -3.21752E-05

NODAL FLUXES FOR FLUID PHASE # 2

NODE	FLUID FLUX	NODE	FLUID FLUX	NODE	FLUID FLUX	NODE	FLUID FLUX	NODE	FLUID FLUX
1	-0.0000E+00	2	-0.0000E+00	41	1.4269E-05	42	1.4269E-05		

SUM OF ABOVE FLUX VALUES = 2.85380E-05

COMPUTATIONAL TIME STEP VALUE = 0.3456E+06 CURRENT TIME = 0.7788E+07

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM HEAD ERROR	NODE NUMBER	MAXIMUM SATUR. ERROR	NODE NUMBER	RELAXATION FACTOR
1	36	-0.9209E-02	23	0.433E-01	17	1.00
2	10	-0.1032E-01	23	0.228E-01	29	1.00
3	4	0.1069E-01	23	0.117E-01	19	0.483
4	4	0.1070E-01	23	0.132E-01	19	1.00
5	10	-0.1715E-01	7	0.174E-01	21	0.312
6	6	-0.1718E-01	7	0.744E-02	31	1.00
7	0	-0.5439E-02	19	0.849E-02	31	1.00

*** NODAL FLUID FLUX VALUES ***

NODAL FLUXES FOR FLUID PHASE # 1

NODE	FLUID FLUX	NODE	FLUID FLUX	NODE	FLUID FLUX	NODE	FLUID FLUX	NODE	FLUID FLUX
1	-1.7202E-05	2	-1.7202E-05	41	1.5850E-06	42	1.5850E-06		

SUM OF ABOVE FLUX VALUES = -3.12335E-05

NODAL FLUXES FOR FLUID PHASE # 2

NODE	FLUID FLUX	NODE	FLUID FLUX	NODE	FLUID FLUX	NODE	FLUID FLUX	NODE	FLUID FLUX
1	-0.0000E+00	2	-0.0000E+00	41	1.4269E-05	42	1.4269E-05		

SUM OF ABOVE FLUX VALUES = 2.85380E-05

*** NODAL PRESSURE VALUES ***

NODE	PRESSURE (Pw)	NODE	PRESSURE (Pw)	NODE	PRESSURE (Pw)	NODE	PRESSURE (Pw)	NODE	PRESSURE (Pw)
1	1.50004E+05	2	1.50004E+05	3	1.47561E+05	4	1.47561E+05	5	1.45057E+05
6	1.45057E+05	7	1.42675E+05	8	1.42675E+05	9	1.40165E+05	10	1.40165E+05
11	1.37781E+05	12	1.37781E+05	13	1.35247E+05	14	1.35247E+05	15	1.32892E+05
16	1.32892E+05	17	1.30467E+05	18	1.30467E+05	19	1.28018E+05	20	1.28018E+05
21	1.25543E+05	22	1.25543E+05	23	1.23075E+05	24	1.23075E+05	25	1.20700E+05
26	1.20700E+05	27	1.18264E+05	28	1.18264E+05	29	1.15768E+05	30	1.15768E+05
31	1.13383E+05	32	1.13383E+05	33	1.10939E+05	34	1.10939E+05	35	1.08496E+05
36	1.08496E+05	37	1.06053E+05	38	1.06053E+05	39	1.03609E+05	40	1.03609E+05
41	1.01136E+05	42	1.01136E+05						

*** NODAL VALUES OF NAPL SATURATION ***

NODE	SATURAT. (Sn)	NODE	SATURAT. (Sn)	NODE	SATURAT. (Sn)	NODE	SATURAT. (Sn)	NODE	SATURAT. (Sn)
1	0.00000E+00	2	0.00000E+00	3	0.00000E+00	4	0.00000E+00	5	0.00000E+00
6	0.00000E+00	7	0.00000E+00	8	0.00000E+00	9	0.00000E+00	10	0.00000E+00
11	0.00000E+00	12	0.00000E+00	13	0.00000E+00	14	0.00000E+00	15	0.00000E+00
16	0.00000E+00	17	1.00557E-02	18	1.00557E-02	19	0.10171	20	0.10171
21	0.12959	22	0.12959	23	0.15167	24	0.15167	25	0.17363
26	0.17363	27	0.19570	28	0.19570	29	0.23175	30	0.23175
31	0.27264	32	0.27264	33	0.32653	34	0.32653	35	0.37621
36	0.37621	37	0.42365	38	0.42365	39	0.46984	40	0.46984
41	0.51273	42	0.51273						

*** NODAL VALUES OF WATER SATURATION ***

NODE	SATURAT. (Sw)	NODE	SATURAT. (Sw)	NODE	SATURAT. (Sw)	NODE	SATURAT. (Sw)	NODE	SATURAT. (Sw)
1	1.0000	2	1.0000	3	1.0000	4	1.0000	5	1.0000
6	1.0000	7	1.0000	8	1.0000	9	1.0000	10	1.0000
11	1.0000	12	1.0000	13	1.0000	14	1.0000	15	1.0000
16	1.0000	17	0.98994	18	0.98994	19	0.89829	20	0.89829
21	0.87041	22	0.87041	23	0.84833	24	0.84833	25	0.82637
26	0.82637	27	0.80430	28	0.80430	29	0.76825	30	0.76825
31	0.72736	32	0.72736	33	0.67347	34	0.67347	35	0.62379
36	0.62379	37	0.57635	38	0.57635	39	0.53016	40	0.53016
41	0.48727	42	0.48727						

*** FLUID FLOW MASS BALANCE INFORMATION AT TIME = 0.7788E+07***

*** MASS BALANCE, FLUID, AND FLOW INFORMATION ***

FLUID PHASE NUMBER 1
NET FLOW RATE DUE TO BOUNDARY FLUX AND SINKS -3.12335E-05
RATE OF FLUID ACCUMULATION -3.00400E-05
MASS BALANCE ERROR -1.19348E-06
NORMALIZED MASS BALANCE ERROR 1.76515E-02
CUMULATIVE FLUID STORAGE -1.97133E+02

*** MASS BALANCE, FLUID, AND FLOW INFORMATION ***

FLUID PHASE NUMBER 2
NET FLOW RATE DUE TO BOUNDARY FLUX AND SINKS 2.85380E-05
RATE OF FLUID ACCUMULATION 2.85380E-05
MASS BALANCE ERROR 3.46280E-14
NORMALIZED MASS BALANCE ERROR 6.06701E-10
CUMULATIVE FLUID STORAGE 2.22253E+02

***** SAMFT2D HAS SOLVED THE PROBLEM *****

*** CPU TIME USED: 20.00 SECS. ***

- 5) Summary of grid specification and boundary condition data;
- 6) Nonlinear iteration summary for each time step;
- 7) For each selected output time value:
 - nodal values of water pressure
 - nodal values of water and NAPL saturations
 - element saturation values and Darcy velocities
 - summary of mass balance information.
- 8) CPU time for the simulation.

10.5 THREE-PHASE FLOW

10.5.1 Input Data

This problem (described in Section 4.4.5) is essentially the same as the problem of section 10.4 except that flow of the air phase is taken into account. The input data file is given in Table 10.7. Except for a few minor alterations, the information in this file is the same as that given in Table 10.5 for the previous input file.

10.5.2 Output

The main output file for the vertical three-phase flow problem is given in Table 10.8.

This output file contains the following information:

- 1) Summary of input control parameters;
- 2) List of automatic time step generation parameters;
- 3) List of default initial condition data;
- 4) List of material properties and tabulated constitutive relations;
- 5) Summary of grid specification and boundary condition data;

Table 10.8 Output for the three-phase flow problem.

THIS OUTPUT GENERATED BY SAMFT2D
 INPUT FILE NAME = 2D10-5.DAT

PROBLEM IDENTIFICATION NUMBER = 1
 PROBLEM EXECUTION INDEX.....(IEXEC) = 1

PROBLEM TITLE

 TEST FOR SAMFT2D,THREE-PHASE VERTICAL FLOW WITH 20-ELEMETS (IFLOW=1)

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
 MATERIAL NUMBER INPUT ? (1=YES,0=NO)(IMNUMR).... = 0
 TOTAL NUMBER OF 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) = 20
 TOTAL NUMBER OF NODES(NP) = 42
 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) = 0
 SEQUENCE OF NODE NUMBERING (0=Y-,1=X-DIR).(ISWAP) = 1

INPUT / OUTPUT CONTROL PARAMETERS

 VELOCITY/INPUT.....(NVREAD) = 0
 BOUNDARY NODE DATA READ (1=YES, 0=NO).....(IOULT) = 1
 NUMBER OF NODES FOR WHICH I.C. ARE READ....(NPIN) = 0
 OUTPUT REQUIREMENT INDICATOR:
 (0=ALL DATA, 1=NO ELEMENT DATA,
 2=NO MESH DATA, 3=NO MESH AND I.C. DATA..(IPRD) = 0
 UNIT 9 OUTPUT (1=YES, 0=NO).....(NVWRIT) = 0
 VELOCITY PRINTOUT CONTROL INDEX.....(NVPR) = 0
 UNIT 10 OUTPUT (0=NONE, N=NTH).....(NPLOT) = 0
 NODAL VALUE PRINTOUT CONTROL INDEX.....(NSTEP) = 10
 OBSERVATION NODE INDEX.....(IOBSND) = 0
 MASS BALANCE TO BE PERFORMED (1=YES,0=NO).(IMBAL) = 1
 UNIT 8 OUTPUT (1=YES, 0=NO).....(NOWRIT) = 1
 PRINT CHECK OPTION INDEX.....(IPRCHK) = 0
 PRESSURE HEAD OUTPUT OPTION INDEX.....(IPWOUT) = 1
 OUTPUT SPECIFIED TIME INDEX.....(NPRCON) = 0

MAX. NUMBER OF NONLINEAR FLOW ITERATIONS..(NITMAX) = 10
 EQUIVALENT FRESHWATER HEAD TOLERANCE.....(HTOL) = 0.1000E-01
 SATURATION TOLERANCE.....(STOL) = 0.1000E-01
 GRAVITATIONAL ACCELERATION.....(GCONST) = 0.9807E+01
 ATMOSPHERIC PRESSURE.....(PATM) = 0.1000E+06
 MAXIMUM NUMBER OF TIME STEP REQUIREMENTS..(IRESOL) = 4

TEMPORAL DISCRETIZATION DATA

 INITIAL TIME VALUE (TIMA) = 0.0000E+00
 VALUE OF FIRST TIME STEP (TIN) = 0.5000E+04
 MINIMUM TIME STEP SIZE..... (TMIN) = 0.1000E+03
 MAXIMUM TIME STEP SIZE (TMAX) = 0.4320E+07
 FINAL TIME VALUE (TEND) = 0.1000E+16

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) = 3
 DEFAULT VALUE OF INITIAL SATURATION OF THE NON-
 AQUEOUS LIQUID PHASE..... HFDAL(1) = 0.0000E+00
 DEFAULT VALUE OF INITIAL PRESSURE OF THE AIR
 PHASE.....HIDAL(2) = 0.1000E+06
 DEPTH FROM SOIL SURFACE TO WATER TABLE..HIDAL(3) = 0.1500E+01

VERTICAL PROFILE FOR INITIAL FUNCTION

CONTROL POINT #	MATERIAL #	VERT. COOR. (+ UPWARD)	FUNCTION VALUE
1	1	0.0000E+00	1.000
2	1	3.500	1.000
3	1	4.875	0.8500

HYDRAULIC PROPERTIES OF POROUS MEDIA

MATERIAL NUMBER: 1 (I)

PERMEABILITY COMPONENT Kxx.....(PROP(I,1)) = 0.0000E+00
 PERMEABILITY COMPONENT Kyy.....(PROP(I,2)) = 0.1000E-11
 PERMEABILITY COMPONENT KXY.....(PROP(I,3)) = 0.0000E+00
 POROUS MATRIX COMPRESSIBILITY (PROP(I,4)) = 0.1000E-09
 EFFECTIVE POROSITY..... (PROP(I,5)) = 0.3000E+00
 AIR ENTRY PRESSURE HEAD..... (PROP(I,6)) = 0.0000E+00

IRREDUCIBLE NAPL SATURATIONSNIRWN(I)= 0.1000E+00
 CRITICAL 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 = 0.1000E-09

FLUID PHASE NUMBER: 2

REFERENCE DENSITY..... = 0.9500E+03
 REFERENCE DYNAMIC VISCOSITY..... = 0.1000E-02
 COMPRESSIBILITY = 0.1000E-09

FLUID PHASE NUMBER: 3

REFERENCE DENSITY..... = 0.1177E+01
 REFERENCE DYNAMIC VISCOSITY..... = 0.1983E-04
 COMPRESSIBILITY = 0.1177E-04

FLUID RETENTION DATA FOR SOIL MATERIAL NO. 1

IRREDUCIBLE WETTING-PHASE SATURATIONPROP(I,7)= 0.2000E+00
 NAPL REL. PERM. AT SWr.....AKSTAR(I)= 0.6800E+00
 N-W CAPILLARY PRESSURE @ SW=1.....PCNSW1(I)= 0.0000E+00

TABULATED REL. PERM. AND CAP. PRESSURE DATA FOR SOIL MATERIAL NO. 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 NO. 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 SPECIFICATION DATA

NUMBER OF ROWS.....(NROWS) = 21
 NUMBER OF COLUMNS.....(NCOLS) = 2
 MAXIMUM ALLOWABLE X-SPACING.....(DXMAX) = 2.00
 MAXIMUM ALLOWABLE Y-SPACING.....(DYMAX) = 0.25
 INPUT INDICATOR FOR GRIDLINE COORD.....(IXYZRD) = 0
 HORIZONTAL PLANE DOMAIN INDICATOR.....(IHORGR) = 0

 X-INCREMENT OF THE FIRST GRID BLOCK(DX) = 2.000
 Y-INCREMENT OF THE FIRST GRID BLOCK(DY) = 0.250
 MAXIMUM VALUE OF X-COORDINATE(X0) = 2.000
 MAXIMUM VALUE OF Y-COORDINATE(Y0) = 5.000
 X-INCREMENT MULTIPLIER(SCFX) = 1.000
 Y-INCREMENT MULTIPLIER(SCFY) = 1.000

MINIMUM VALUE OF X-COORDINATE(XSTART) = 0.000
 MINIMUM VALUE OF Y-COORDINATE(YSTART) = 0.000

*** FINITE-ELEMENT MESH NODAL CONNECTIONS ***

 (NUMBERING IS COUNTER-CLOCKWISE)

ELEMENT	ELEMENTAL NODE NUMBERING					ELEMENT	ELEMENTAL NODE NUMBERING				
-----	-----					-----	-----				
1	1	2	4	3	2	3	4	6	5		
3	5	6	8	7	4	7	8	10	9		
5	9	10	12	11	6	11	12	14	13		
7	13	14	16	15	8	15	16	18	17		
9	17	18	20	19	10	19	20	22	21		
11	21	22	24	23	12	23	24	26	25		
13	25	26	28	27	14	27	28	30	29		
15	29	30	32	31	16	31	32	34	33		
17	33	34	36	35	18	35	36	38	37		
19	37	38	40	39	20	39	40	42	41		

*** NODAL COORDINATES ***

NODE	X-COOR.	Y-COOR.	NODE	X-COOR.	Y-COOR.
----	-----	-----	----	-----	-----
1	0.00	0.00	2	2.00	0.00
3	0.00	0.25	4	2.00	0.25
5	0.00	0.50	6	2.00	0.50
7	0.00	0.75	8	2.00	0.75
9	0.00	1.00	10	2.00	1.00
11	0.00	1.25	12	2.00	1.25
13	0.00	1.50	14	2.00	1.50
15	0.00	1.75	16	2.00	1.75
17	0.00	2.00	18	2.00	2.00
19	0.00	2.25	20	2.00	2.25
21	0.00	2.50	22	2.00	2.50
23	0.00	2.75	24	2.00	2.75
25	0.00	3.00	26	2.00	3.00
27	0.00	3.25	28	2.00	3.25
29	0.00	3.50	30	2.00	3.50
31	0.00	3.75	32	2.00	3.75
33	0.00	4.00	34	2.00	4.00
35	0.00	4.25	36	2.00	4.25
37	0.00	4.50	38	2.00	4.50
39	0.00	4.75	40	2.00	4.75
41	0.00	5.00	42	2.00	5.00

BOUNDARY CONDITION DATA

 NUMBER OF STEADY DIRICHLET BOUNDARIES (NBTO) = 6
 NUMBER OF STEADY FLUX BOUNDARIES (NDFLUX) = 4
 NUMBER OF TRANSIENT DIRICHLET BOUNDARIES.... (NBHVAR) = 0
 NUMBER OF TRANSIENT FLUX BOUNDARIES..... (NBFVAR) = 0

STEADY-STATE DIRICHLET BOUNDARY CONDITIONS

INDEX	NODE NO.	D.V. NO.	PRESCRIBED VALUE	B.C. IDENTIFIER
1	1	1	150000.	-1
2	1	2	150000.	-1
3	1	3	150000.	-1
4	2	1	150000.	-1
5	2	2	150000.	-1
6	2	3	150000.	-1

STEADY-STATE FLUX BOUNDARY CONDITIONS

INDEX	NODE NO.	D.V. NO.	FLUID FLUX VALUE
1	41	1	3.170900E-06
2	41	2	2.853800E-05
3	42	1	3.170900E-06
4	42	2	2.853800E-05

 * INITIAL CONDITION FOR FLOW PROBLEM *

NODE	PRES. (PH.1)	SAT. (PH. 1)	SAT. (PH. 2)	PRES. (PH. 2)	SAT. (PH. 3)	PRES. (PH.3)
1	0.134323E+06	0.1000E+01	0.0000E+00	0.134323E+06	0.0000E+00	0.100000E+06
3	0.131871E+06	0.1000E+01	0.0000E+00	0.131871E+06	0.0000E+00	0.100000E+06
5	0.129420E+06	0.1000E+01	0.0000E+00	0.129420E+06	0.0000E+00	0.100000E+06
7	0.126968E+06	0.1000E+01	0.0000E+00	0.126968E+06	0.0000E+00	0.100000E+06
9	0.124517E+06	0.1000E+01	0.0000E+00	0.124517E+06	0.0000E+00	0.100000E+06
11	0.122065E+06	0.1000E+01	0.0000E+00	0.122065E+06	0.0000E+00	0.100000E+06
13	0.119613E+06	0.1000E+01	0.0000E+00	0.119613E+06	0.0000E+00	0.100000E+06
15	0.117162E+06	0.1000E+01	0.0000E+00	0.117162E+06	0.0000E+00	0.100000E+06
17	0.114710E+06	0.1000E+01	0.0000E+00	0.114710E+06	0.0000E+00	0.100000E+06
19	0.112258E+06	0.1000E+01	0.0000E+00	0.112258E+06	0.0000E+00	0.100000E+06
21	0.109807E+06	0.1000E+01	0.0000E+00	0.109807E+06	0.0000E+00	0.100000E+06
23	0.107355E+06	0.1000E+01	0.0000E+00	0.107355E+06	0.0000E+00	0.100000E+06
25	0.104903E+06	0.1000E+01	0.0000E+00	0.104903E+06	0.0000E+00	0.100000E+06
27	0.102452E+06	0.1000E+01	0.0000E+00	0.102452E+06	0.0000E+00	0.100000E+06
29	0.100000E+06	0.1000E+01	0.0000E+00	0.100000E+06	0.0000E+00	0.100000E+06
31	0.997273E+05	0.9727E+00	0.0000E+00	0.997273E+05	0.2727E-01	0.100000E+06
33	0.994545E+05	0.9455E+00	0.0000E+00	0.994545E+05	0.5455E-01	0.100000E+06
35	0.991818E+05	0.9182E+00	0.0000E+00	0.991818E+05	0.8182E-01	0.100000E+06
37	0.989091E+05	0.8909E+00	0.0000E+00	0.989091E+05	0.1091E+00	0.100000E+06
39	0.986364E+05	0.8636E+00	0.0000E+00	0.986364E+05	0.1364E+00	0.100000E+06
41	0.983636E+05	0.8364E+00	0.0000E+00	0.983636E+05	0.1636E+00	0.100000E+06
2	0.134323E+06	0.1000E+01	0.0000E+00	0.134323E+06	0.0000E+00	0.100000E+06
4	0.131871E+06	0.1000E+01	0.0000E+00	0.131871E+06	0.0000E+00	0.100000E+06
6	0.129420E+06	0.1000E+01	0.0000E+00	0.129420E+06	0.0000E+00	0.100000E+06
8	0.126968E+06	0.1000E+01	0.0000E+00	0.126968E+06	0.0000E+00	0.100000E+06
10	0.124517E+06	0.1000E+01	0.0000E+00	0.124517E+06	0.0000E+00	0.100000E+06
12	0.122065E+06	0.1000E+01	0.0000E+00	0.122065E+06	0.0000E+00	0.100000E+06
14	0.119613E+06	0.1000E+01	0.0000E+00	0.119613E+06	0.0000E+00	0.100000E+06
16	0.117162E+06	0.1000E+01	0.0000E+00	0.117162E+06	0.0000E+00	0.100000E+06
18	0.114710E+06	0.1000E+01	0.0000E+00	0.114710E+06	0.0000E+00	0.100000E+06
20	0.112258E+06	0.1000E+01	0.0000E+00	0.112258E+06	0.0000E+00	0.100000E+06
22	0.109807E+06	0.1000E+01	0.0000E+00	0.109807E+06	0.0000E+00	0.100000E+06
24	0.107355E+06	0.1000E+01	0.0000E+00	0.107355E+06	0.0000E+00	0.100000E+06
26	0.104903E+06	0.1000E+01	0.0000E+00	0.104903E+06	0.0000E+00	0.100000E+06

28	0.102452E+06	0.1000E+01	0.0000E+00	0.102452E+06	0.0000E+00	0.100000E+06
30	0.100000E+06	0.1000E+01	0.0000E+00	0.100000E+06	0.0000E+00	0.100000E+06
32	0.997273E+05	0.9727E+00	0.0000E+00	0.997273E+05	0.2727E-01	0.100000E+06
34	0.994545E+05	0.9455E+00	0.0000E+00	0.994545E+05	0.5455E-01	0.100000E+06
36	0.991818E+05	0.9182E+00	0.0000E+00	0.991818E+05	0.8182E-01	0.100000E+06
38	0.989091E+05	0.8909E+00	0.0000E+00	0.989091E+05	0.1091E+00	0.100000E+06
40	0.986364E+05	0.8636E+00	0.0000E+00	0.986364E+05	0.1364E+00	0.100000E+06
42	0.983636E+05	0.8364E+00	0.0000E+00	0.983636E+05	0.1636E+00	0.100000E+06

LIST OF BOUNDARY NODE NUMBERS

 1 2 41 42

DISTANCE SCALE FACTOR FOR PRESSURE B.C.INCORPORATION = 0.80000E+01

MATRIX BANDWIDTH REQUIRED FOR FLOW SIMULATION = 23
 =====

+++++++ BEGIN TRANSIENT CALCULATIONS ++++++

 *** ELAPSED TIME: 5000. TIME STEP: 1 TIME STEP SIZE: 0.500E+04 ***

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM HEAD ERROR	NODE NUMBER	MAXIMUM SATUR. ERROR	NODE NUMBER	RELAXATION FACTOR
-----	-----	-----	-----	-----	-----	-----
1	56	0.6774	7	0.140	41	1.00
2	56	0.3024	1	0.732E-01	29	1.00
3	46	-0.5767E-01	1	0.186E-01	31	0.880
4	0	-0.9530E-02	5	0.432E-02	31	1.00

 *** ELAPSED TIME: 0.1078E+05 TIME STEP: 2 TIME STEP SIZE: 0.578E+04 ***

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM HEAD ERROR	NODE NUMBER	MAXIMUM SATUR. ERROR	NODE NUMBER	RELAXATION FACTOR
-----	-----	-----	-----	-----	-----	-----
1	52	0.1524	5	0.107	41	1.00
2	0	-0.3808E-02	41	0.369E-02	37	0.983

 *** ELAPSED TIME: 0.2103E+05 TIME STEP: 3 TIME STEP SIZE: 0.103E+05 ***

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM HEAD ERROR	NODE NUMBER	MAXIMUM SATUR. ERROR	NODE NUMBER	RELAXATION FACTOR
1	50	0.1478	31	0.740E-01	41	1.00
2	0	-0.2368E-02	41	0.575E-02	41	0.989

 *** ELAPSED TIME: 0.4435E+05 TIME STEP: 4 TIME STEP SIZE: 0.233E+05 ***

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM HEAD ERROR	NODE NUMBER	MAXIMUM SATUR. ERROR	NODE NUMBER	RELAXATION FACTOR
1	48	0.2557	41	0.287E-01	41	1.00
2	0	0.3799E-02	35	0.375E-02	35	1.00

 *** ELAPSED TIME: 0.1417E+06 TIME STEP: 5 TIME STEP SIZE: 0.973E+05 ***

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM HEAD ERROR	NODE NUMBER	MAXIMUM SATUR. ERROR	NODE NUMBER	RELAXATION FACTOR
1	52	1.202	41	0.127	35	1.00
2	46	-0.8462	41	0.120	35	0.620
3	48	-0.3374	41	0.517E-01	35	1.00
4	0	0.1020E-02	41	0.514E-02	41	0.998

 *** ELAPSED TIME: 0.2892E+06 TIME STEP: 6 TIME STEP SIZE: 0.148E+06 ***

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM HEAD ERROR	NODE NUMBER	MAXIMUM SATUR. ERROR	NODE NUMBER	RELAXATION FACTOR
1	10	0.3973E-01	41	0.118	41	1.00
2	4	0.2223E-01	39	0.167E-01	41	1.00
3	0	0.2754E-02	35	0.279E-02	37	1.00

 *** ELAPSED TIME: 0.4872E+06 TIME STEP: 7 TIME STEP SIZE: 0.198E+06 ***

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM HEAD ERROR	NODE NUMBER	MAXIMUM SATUR. ERROR	NODE NUMBER	RELAXATION FACTOR
1	12	0.2082	39	0.779E-01	39	1.00

2	10	-0.1134E-01	39	0.264E-01	39	0.964
3	0	-0.5786E-02	35	0.437E-02	37	1.00

 *** ELAPSED TIME: 0.7696E+06 TIME STEP: 8 TIME STEP SIZE: 0.282E+06 ***

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM HEAD ERROR	NODE NUMBER	MAXIMUM SATUR. ERROR	NODE NUMBER	RELAXATION FACTOR
1	18	0.2650	39	0.158	39	1.00
2	22	-0.1846	39	0.602E-01	39	0.623
3	24	-0.2573	37	0.244	41	0.819
4	30	0.1876	37	0.118	41	0.542
5	34	0.8597E-01	37	0.952E-01	41	1.00
6	8	-0.1170E-01	13	0.194E-01	41	0.913
7	2	-0.1024E-01	9	0.252E-02	41	1.00
8	0	-0.9680E-02	7	0.244E-02	41	1.00

 *** ELAPSED TIME: 0.1085E+07 TIME STEP: 9 TIME STEP SIZE: 0.316E+06 ***

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM HEAD ERROR	NODE NUMBER	MAXIMUM SATUR. ERROR	NODE NUMBER	RELAXATION FACTOR
1	12	0.3131E-01	39	0.125	39	1.00
2	12	0.1141	37	0.566E-01	37	1.00
3	10	0.6096E-01	37	0.566E-01	39	1.00
4	6	0.1556E-01	5	0.184E-01	37	1.00
5	2	0.1168E-01	3	0.364E-02	41	1.00
6	0	-0.9737E-02	21	0.355E-02	41	0.565

 *** ELAPSED TIME: 0.1382E+07 TIME STEP: 10 TIME STEP SIZE: 0.297E+06 ***

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM HEAD ERROR	NODE NUMBER	MAXIMUM SATUR. ERROR	NODE NUMBER	RELAXATION FACTOR
1	12	0.6778E-01	37	0.117	37	1.00
2	18	-0.2426E-01	37	0.702E-01	37	0.787
3	12	0.8316E-01	35	0.251E-01	37	0.115
4	12	0.8298E-01	35	0.251E-01	37	1.00
5	2	0.2550E-01	35	0.807E-02	35	1.00
6	4	0.1552E-01	35	0.525E-02	35	1.00
7	0	0.9336E-02	21	0.364E-02	37	1.00

*** NODAL FLUID FLUX VALUES ***

NODAL FLUXES FOR FLUID PHASE # 1

NODE	FLUID FLUX	NODE	FLUID FLUX	NODE	FLUID FLUX	NODE	FLUID FLUX	NODE	FLUID FLUX
1	-3.3196E-05	2	-3.3196E-05	41	3.1709E-06	42	3.1709E-06		

SUM OF ABOVE FLUX VALUES = -6.00495E-05

NODAL FLUXES FOR FLUID PHASE # 2

NODE	FLUID FLUX	NODE	FLUID FLUX	NODE	FLUID FLUX	NODE	FLUID FLUX	NODE	FLUID FLUX
1	0.0000E+00	2	0.0000E+00	41	2.8538E-05	42	2.8538E-05		

SUM OF ABOVE FLUX VALUES = 5.70760E-05

*** NODAL PRESSURE VALUES ***

NODE	PRESSURE (Pn)	NODE	PRESSURE (Pn)	NODE	PRESSURE (Pn)	NODE	PRESSURE (Pn)	NODE	PRESSURE (Pn)
1	1.50004E+05	2	1.50004E+05	3	1.47561E+05	4	1.47561E+05	5	1.45119E+05
6	1.45119E+05	7	1.42676E+05	8	1.42676E+05	9	1.40234E+05	10	1.40234E+05
11	1.37791E+05	12	1.37791E+05	13	1.35344E+05	14	1.35344E+05	15	1.32901E+05
16	1.32901E+05	17	1.30473E+05	18	1.30473E+05	19	1.28032E+05	20	1.28032E+05
21	1.25571E+05	22	1.25571E+05	23	1.23138E+05	24	1.23138E+05	25	1.20696E+05
26	1.20696E+05	27	1.18254E+05	28	1.18254E+05	29	1.15811E+05	30	1.15811E+05
31	1.13369E+05	32	1.13369E+05	33	1.10927E+05	34	1.10927E+05	35	1.09720E+05
36	1.09720E+05	37	1.07917E+05	38	1.07917E+05	39	1.06659E+05	40	1.06659E+05
41	1.06026E+05	42	1.06026E+05						

*** NODAL VALUES OF NAPL SATURATION ***

NODE	SATURAT. (Sn)	NODE	SATURAT. (Sn)	NODE	SATURAT. (Sn)	NODE	SATURAT. (Sn)	NODE	SATURAT. (Sn)
1	0.00000E+00	2	0.00000E+00	3	0.00000E+00	4	0.00000E+00	5	0.00000E+00
6	0.00000E+00	7	0.00000E+00	8	0.00000E+00	9	0.00000E+00	10	0.00000E+00
11	0.00000E+00	12	0.00000E+00	13	0.00000E+00	14	0.00000E+00	15	0.00000E+00
16	0.00000E+00	17	0.00000E+00	18	0.00000E+00	19	0.00000E+00	20	0.00000E+00
21	0.00000E+00	22	0.00000E+00	23	0.00000E+00	24	0.00000E+00	25	0.00000E+00
26	0.00000E+00	27	0.00000E+00	28	0.00000E+00	29	0.00000E+00	30	0.00000E+00
31	0.00000E+00	32	0.00000E+00	33	0.00000E+00	34	0.00000E+00	35	9.05326E-02
36	9.05326E-02	37	0.13511	38	0.13511	39	0.21484	40	0.21484
41	0.22626	42	0.22626						

*** NODAL VALUES OF WATER SATURATION ***

NODE	SATURAT. (SW)	NODE	SATURAT. (SW)	NODE	SATURAT. (SW)	NODE	SATURAT. (SW)	NODE	SATURAT. (SW)
1	1.0000	2	1.0000	3	1.0000	4	1.0000	5	1.0000
6	1.0000	7	1.0000	8	1.0000	9	1.0000	10	1.0000
11	1.0000	12	1.0000	13	1.0000	14	1.0000	15	1.0000
16	1.0000	17	1.0000	18	1.0000	19	1.0000	20	1.0000
21	1.0000	22	1.0000	23	1.0000	24	1.0000	25	1.0000
26	1.0000	27	1.0000	28	1.0000	29	1.0000	30	1.0000
31	1.0012	32	1.0012	33	1.0005	34	1.0005	35	0.90963
36	0.90963	37	0.85796	38	0.85796	39	0.55664	40	0.55664
41	0.33124	42	0.33124						

*** FLUID FLOW MASS BALANCE INFORMATION AT TIME = 0.1382E+07***

*** MASS BALANCE, FLUID, AND FLOW INFORMATION ***

FLUID PHASE NUMBER 1
NET FLOW RATE DUE TO BOUNDARY FLUX AND SINKS -6.00495E-05
RATE OF FLUID ACCUMULATION -6.00495E-05
MASS BALANCE ERROR -1.62407E-16
NORMALIZED MASS BALANCE ERROR 1.22310E-12
CUMULATIVE FLUID STORAGE -7.76353E+01

*** MASS BALANCE, FLUID, AND FLOW INFORMATION ***

FLUID PHASE NUMBER 2
NET FLOW RATE DUE TO BOUNDARY FLUX AND SINKS 5.70760E-05
RATE OF FLUID ACCUMULATION 5.70760E-05
MASS BALANCE ERROR -1.35525E-20
NORMALIZED MASS BALANCE ERROR 1.18724E-16
CUMULATIVE FLUID STORAGE 7.88892E+01

*** ELAPSED TIME: 0.1710E+07 TIME STEP: 11 TIME STEP SIZE: 0.328E+06 ***

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM HEAD ERROR	NODE NUMBER	MAXIMUM SATUR. ERROR	NODE NUMBER	RELAXATION FACTOR
1	14	0.2263	35	0.783E-01	35	1.00
2	18	-0.1762	35	0.121	33	0.588
3	14	0.8357E-01	33	0.180E-01	37	0.576
4	14	-0.3596E-01	35	0.178E-01	35	0.601
5	12	-0.2204E-01	35	0.202E-01	37	1.00
6	10	0.3889E-01	33	0.128E-01	37	0.283
7	8	0.2064E-01	33	0.122E-01	37	1.00
8	0	0.4941E-02	25	0.334E-02	37	1.00

 *** ELAPSED TIME: 0.2121E+07 TIME STEP: 12 TIME STEP SIZE: 0.411E+06 ***

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM HEAD ERROR	NODE NUMBER	MAXIMUM SATUR. ERROR	NODE NUMBER	RELAXATION FACTOR
1	18	0.2158	33	0.849E-01	33	1.00
2	22	-0.1396	33	0.143	31	0.645
3	20	0.7058E-01	31	0.235E-01	37	0.586
4	24	0.2834E-01	31	0.190E-01	35	1.00
5	2	0.1872E-01	31	0.794E-02	31	1.00
6	4	0.1662E-01	29	0.630E-02	37	1.00
7	10	0.1722E-01	27	0.199E-01	37	1.00
8	2	-0.1975E-01	31	0.817E-02	31	0.436
9	2	-0.1742E-01	31	0.721E-02	31	1.00
10	2	0.1580E-01	31	0.805E-02	35	0.536

..... SOLUTION NOT CONVERGING.....
 WORST HEAD ERROR = 0.1580E-01
 WORST SATURATION ERROR = 0.8052E-02

COMPUTATIONAL TIME STEP VALUE = 0.4107E+05 CURRENT TIME = 0.1751E+07

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM HEAD ERROR	NODE NUMBER	MAXIMUM SATUR. ERROR	NODE NUMBER	RELAXATION FACTOR
1	6	0.2490E-01	33	0.101E-01	33	1.00
2	0	-0.5589E-02	31	0.212E-02	41	0.861

COMPUTATIONAL TIME STEP VALUE = 0.2053E+06 CURRENT TIME = 0.1956E+07

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM HEAD ERROR	NODE NUMBER	MAXIMUM SATUR. ERROR	NODE NUMBER	RELAXATION FACTOR
1	18	0.9360E-01	33	0.331E-01	33	1.00
2	10	-0.5409E-01	33	0.242E-01	31	0.677
3	8	-0.1800E-01	33	0.202E-01	31	1.00
4	4	-0.1597E-01	19	0.651E-02	35	1.00
5	6	0.1371E-01	29	0.446E-02	35	0.555
6	6	0.1371E-01	29	0.387E-02	35	1.00
7	6	0.1260E-01	37	0.116E-01	37	1.00
8	6	0.1076E-01	31	0.116E-01	31	1.00
9	0	0.9076E-02	35	0.880E-02	35	1.00

COMPUTATIONAL TIME STEP VALUE = 0.1643E+06 CURRENT TIME = 0.2121E+07

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM HEAD ERROR	NODE NUMBER	MAXIMUM SATUR. ERROR	NODE NUMBER	RELAXATION FACTOR
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1	8	0.5803E-01	31	0.448E-01	31	1.00
2	10	-0.1256E-01	31	0.151E-01	31	0.865
3	0	0.9240E-02	9	0.659E-02	33	0.558

 *** ELAPSED TIME: 0.2630E+07 TIME STEP: 13 TIME STEP SIZE: 0.510E+06 ***

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM HEAD ERROR	NODE NUMBER	MAXIMUM SATUR. ERROR	NODE NUMBER	RELAXATION FACTOR
1	26	0.2563	31	0.117	31	1.00
2	28	-0.1497	31	0.177	29	0.674
3	32	0.1085	29	0.724E-01	29	0.465
4	18	0.3678E-01	29	0.235E-01	31	1.00
5	22	0.1725E-01	37	0.218E-01	31	1.00
6	2	0.1791E-01	29	0.840E-02	37	1.00
7	4	0.1299E-01	29	0.540E-02	37	1.00
8	4	-0.1358E-01	29	0.904E-02	37	0.478
9	2	-0.1013E-01	29	0.409E-02	29	1.00
10	2	0.1336E-01	29	0.543E-02	29	0.379

..... SOLUTION NOT CONVERGING.....
 WORST HEAD ERROR = 0.1336E-01
 WORST SATURATION ERROR = 0.5431E-02

COMPUTATIONAL TIME STEP VALUE = 0.5096E+05 CURRENT TIME = 0.2172E+07

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM HEAD ERROR	NODE NUMBER	MAXIMUM SATUR. ERROR	NODE NUMBER	RELAXATION FACTOR
1	8	0.2924E-01	31	0.121E-01	31	1.00
2	0	0.4653E-02	33	0.210E-02	35	1.00

COMPUTATIONAL TIME STEP VALUE = 0.2548E+06 CURRENT TIME = 0.2427E+07

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM HEAD ERROR	NODE NUMBER	MAXIMUM SATUR. ERROR	NODE NUMBER	RELAXATION FACTOR
1	24	0.1209	31	0.471E-01	31	1.00
2	16	-0.6030E-01	31	0.385E-01	29	0.715
3	8	-0.2029E-01	31	0.105E-01	31	1.00
4	2	0.1004E-01	5	0.365E-02	39	0.717
5	4	-0.1402E-01	7	0.338E-02	39	0.257
6	4	-0.1402E-01	7	0.329E-02	39	1.00
7	6	-0.1762E-01	41	0.127E-01	39	1.00
8	2	0.1264E-01	3	0.168E-02	29	0.614
9	2	0.1264E-01	3	0.131E-02	31	1.00
10	0	-0.7760E-02	3	0.123E-02	31	0.660

COMPUTATIONAL TIME STEP VALUE = 0.2038E+06 CURRENT TIME = 0.2630E+07

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM HEAD ERROR	NODE NUMBER	MAXIMUM SATUR. ERROR	NODE NUMBER	RELAXATION FACTOR
1	8	0.6717E-01	29	0.529E-01	29	1.00
2	10	-0.1535E-01	29	0.193E-01	29	0.858
3	2	0.1323E-01	31	0.818E-02	31	0.498
4	4	0.1643E-01	29	0.465E-02	31	1.00
5	2	-0.1344E-01	29	0.424E-02	33	0.571
6	2	-0.1256E-01	29	0.343E-02	33	1.00
7	2	0.1169E-01	35	0.763E-02	33	0.526
8	4	0.1765E-01	5	0.713E-02	33	1.00
9	2	0.1078E-01	29	0.502E-02	35	1.00
10	0	-0.8757E-02	29	0.521E-02	33	0.574

 *** ELAPSED TIME: 0.3203E+07 TIME STEP: 14 TIME STEP SIZE: 0.572E+06 ***

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM HEAD ERROR	NODE NUMBER	MAXIMUM SATUR. ERROR	NODE NUMBER	RELAXATION FACTOR
1	32	0.2534	29	0.107	29	1.00
2	34	-0.1627	29	0.206	27	0.647
3	34	0.1061	27	0.873E-01	27	0.496
4	20	-0.3687E-01	29	0.229E-01	29	0.622
5	20	-0.2122E-01	29	0.211E-01	29	1.00
6	8	0.2081E-01	27	0.649E-02	41	0.507
7	6	-0.1662E-01	15	0.671E-02	29	0.318
8	2	-0.1142E-01	21	0.659E-02	29	1.00
9	8	-0.3192E-01	27	0.101E-01	37	1.00
10	6	0.2979E-01	27	0.111E-01	37	0.525

..... SOLUTION NOT CONVERGING.....
 WORST HEAD ERROR = 0.2979E-01
 WORST SATURATION ERROR = 0.1106E-01

COMPUTATIONAL TIME STEP VALUE = 0.5725E+05 CURRENT TIME = 0.2688E+07

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM HEAD ERROR	NODE NUMBER	MAXIMUM SATUR. ERROR	NODE NUMBER	RELAXATION FACTOR
1	8	0.2258E-01	29	0.103E-01	29	1.00
2	0	-0.9785E-02	11	0.300E-02	41	0.748

COMPUTATIONAL TIME STEP VALUE = 0.2862E+06 CURRENT TIME = 0.2974E+07

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM HEAD ERROR	NODE NUMBER	MAXIMUM SATUR. ERROR	NODE NUMBER	RELAXATION FACTOR
1	26	0.1042	29	0.389E-01	29	1.00
2	10	-0.5162E-01	29	0.307E-01	27	0.716

3	4	-0.1687E-01	29	0.759E-02	29	1.00
4	6	0.1315E-01	19	0.239E-02	31	0.588
5	6	0.1315E-01	19	0.641E-02	31	1.00
6	2	0.1569E-01	39	0.487E-02	31	1.00
7	2	0.1504E-01	3	0.619E-02	27	1.00
8	0	0.7723E-02	19	0.386E-02	31	1.00

COMPUTATIONAL TIME STEP VALUE = 0.2290E+06 CURRENT TIME = 0.3203E+07

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM HEAD ERROR	NODE NUMBER	MAXIMUM SATUR. ERROR	NODE NUMBER	RELAXATION FACTOR
1	12	0.4159E-01	27	0.486E-01	27	1.00
2	4	0.9540E-02	25	0.154E-01	27	1.00
3	0	-0.9535E-02	25	0.629E-02	29	0.500

 *** ELAPSED TIME: 0.3929E+07 TIME STEP: 15 TIME STEP SIZE: 0.727E+06 ***

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM HEAD ERROR	NODE NUMBER	MAXIMUM SATUR. ERROR	NODE NUMBER	RELAXATION FACTOR
1	40	0.2761	27	0.133	27	1.00
2	42	-0.1507	27	0.267	25	0.692
3	42	0.1136	25	0.134	25	0.459
4	44	0.7009E-01	25	0.661E-01	25	1.00
5	28	-0.2072E-01	27	0.275E-01	27	0.821
6	2	-0.1062E-01	9	0.686E-02	33	1.00
7	0	0.9098E-02	39	0.823E-02	39	0.556

 *** ELAPSED TIME: 0.4781E+07 TIME STEP: 16 TIME STEP SIZE: 0.851E+06 ***

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM HEAD ERROR	NODE NUMBER	MAXIMUM SATUR. ERROR	NODE NUMBER	RELAXATION FACTOR
1	42	0.2788	25	0.111	25	1.00
2	46	-0.2003	25	0.337	23	0.593
3	44	0.1173	23	0.142	23	0.505
4	42	0.6582E-01	23	0.638E-01	23	1.00
5	12	-0.1634E-01	25	0.273E-01	23	0.847
6	4	-0.6677E-02	21	0.115E-01	33	1.00
7	0	-0.6695E-02	21	0.832E-02	33	1.00

 *** ELAPSED TIME: 0.5693E+07 TIME STEP: 17 TIME STEP SIZE: 0.913E+06 ***

NUMBER OF MAXIMUM MAXIMUM

ITERATION	NON-CONVERGENT NODES	HEAD ERROR	NODE NUMBER	SATUR. ERROR	NODE NUMBER	RELAXATION FACTOR
1	48	0.1983	23	0.705E-01	23	1.00
2	52	-0.1525	23	0.299	21	0.592
3	40	0.1178	21	0.116	21	0.383
4	36	0.5865E-01	21	0.815E-01	21	1.00
5	22	0.1868E-01	39	0.396E-01	21	1.00
6	8	0.2742E-01	21	0.500E-02	27	1.00
7	12	-0.1291E-01	21	0.449E-02	21	0.729
8	12	-0.1128E-01	25	0.388E-02	21	1.00
9	0	-0.9283E-02	19	0.404E-02	31	1.00

 *** ELAPSED TIME: 0.6707E+07 TIME STEP: 18 TIME STEP SIZE: 0.101E+07 ***

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM HEAD ERROR	NODE NUMBER	MAXIMUM SATUR. ERROR	NODE NUMBER	RELAXATION FACTOR
1	58	0.1533	21	0.563E-01	21	1.00
2	58	-0.1094	21	0.264	19	0.616
3	34	0.1270	19	0.952E-01	19	0.265
4	32	-0.6126E-01	21	0.104	19	0.275
5	38	0.9326E-01	19	0.371E-01	19	0.903E-01
6	30	0.9298E-01	19	0.364E-01	19	1.00
7	16	0.1322E-01	17	0.276E-01	19	1.00
8	6	-0.1309E-01	13	0.102E-01	29	0.504
9	2	-0.1309E-01	13	0.849E-02	29	1.00
10	8	-0.1385E-01	41	0.184E-01	39	1.00

..... SOLUTION NOT CONVERGING.....
 WORST HEAD ERROR = -0.1385E-01
 WORST SATURATION ERROR = 0.1843E-01

COMPUTATIONAL TIME STEP VALUE = 0.1014E+06 CURRENT TIME = 0.5795E+07

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM HEAD ERROR	NODE NUMBER	MAXIMUM SATUR. ERROR	NODE NUMBER	RELAXATION FACTOR
1	2	0.2352E-01	21	0.825E-02	21	1.00
2	0	0.7496E-02	41	0.690E-02	41	1.00

COMPUTATIONAL TIME STEP VALUE = 0.5070E+06 CURRENT TIME = 0.6302E+07

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM HEAD ERROR	NODE NUMBER	MAXIMUM SATUR. ERROR	NODE NUMBER	RELAXATION FACTOR
1	48	0.5759E-01	21	0.305E-01	31	1.00
2	16	-0.4313E-01	21	0.442E-01	19	0.600
3	14	0.3843E-01	19	0.331E-01	19	0.337
4	6	-0.1926E-01	21	0.110E-01	19	0.336

5	6	0.3247E-01	19	0.198E-01	19	0.997E-01
6	6	0.3107E-01	19	0.186E-01	19	1.00
7	0	0.6738E-02	25	0.660E-02	25	1.00

COMPUTATIONAL TIME STEP VALUE = 0.4056E+06 CURRENT TIME = 0.6707E+07

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM HEAD ERROR	NODE NUMBER	MAXIMUM SATUR. ERROR	NODE NUMBER	RELAXATION FACTOR
1	32	0.9619E-01	19	0.561E-01	19	1.00
2	22	0.2499E-01	21	0.266E-01	17	1.00
3	14	-0.1983E-01	19	0.266E-01	17	0.582
4	4	0.9770E-02	13	0.111E-01	17	0.560
5	0	-0.9214E-02	41	0.502E-02	39	0.297

 *** ELAPSED TIME: 0.7767E+07 TIME STEP: 19 TIME STEP SIZE: 0.106E+07 ***

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM HEAD ERROR	NODE NUMBER	MAXIMUM SATUR. ERROR	NODE NUMBER	RELAXATION FACTOR
1	66	0.1276	19	0.546E-01	29	1.00
2	56	-0.9647E-01	19	0.227	17	0.597
3	16	0.1270	17	0.651E-01	17	0.227
4	34	0.6284E-01	17	0.760E-01	17	1.00
5	30	-0.2907E-01	15	0.553E-01	17	0.733
6	14	0.2197E-01	17	0.118E-01	15	0.485
7	6	0.2248E-01	15	0.607E-02	15	1.00
8	0	-0.9812E-02	15	0.376E-02	27	0.746

 *** ELAPSED TIME: 0.8896E+07 TIME STEP: 20 TIME STEP SIZE: 0.113E+07 ***

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM HEAD ERROR	NODE NUMBER	MAXIMUM SATUR. ERROR	NODE NUMBER	RELAXATION FACTOR
1	64	0.1192	17	0.655E-01	27	1.00
2	42	-0.7768E-01	17	0.220	15	0.643
3	14	0.1281	15	0.723E-01	15	0.195
4	38	0.5576E-01	15	0.928E-01	15	1.00
5	40	-0.5666E-01	13	0.743E-01	15	0.492
6	32	0.4457E-01	15	0.282E-01	13	0.313
7	28	0.2649E-01	15	0.194E-01	13	1.00
8	2	0.1158E-01	7	0.103E-02	15	1.00
9	2	-0.1251E-01	11	0.853E-03	15	0.463
10	2	-0.1251E-01	11	0.796E-03	15	1.00

..... SOLUTION NOT CONVERGING.....
 WORST HEAD ERROR = -0.1251E-01
 WORST SATURATION ERROR = 0.7963E-03

COMPUTATIONAL TIME STEP VALUE = 0.1129E+06 CURRENT TIME = 0.7880E+07

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM HEAD ERROR	NODE NUMBER	MAXIMUM SATUR. ERROR	NODE NUMBER	RELAXATION FACTOR
1	8	0.1783E-01	21	0.985E-02	27	1.00
2	0	-0.6530E-02	3	0.575E-02	19	0.782

*** NODAL FLUID FLUX VALUES ***

NODAL FLUXES FOR FLUID PHASE # 1

NODE	FLUID FLUX	NODE	FLUID FLUX	NODE	FLUID FLUX	NODE	FLUID FLUX	NODE	FLUID FLUX
1	-3.3339E-05	2	-3.3339E-05	41	3.1709E-06	42	3.1709E-06		

SUM OF ABOVE FLUX VALUES = -6.03365E-05

NODAL FLUXES FOR FLUID PHASE # 2

NODE	FLUID FLUX	NODE	FLUID FLUX	NODE	FLUID FLUX	NODE	FLUID FLUX	NODE	FLUID FLUX
1	0.0000E+00	2	0.0000E+00	41	2.8538E-05	42	2.8538E-05		

SUM OF ABOVE FLUX VALUES = 5.70760E-05

COMPUTATIONAL TIME STEP VALUE = 0.5647E+06 CURRENT TIME = 0.8445E+07

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM HEAD ERROR	NODE NUMBER	MAXIMUM SATUR. ERROR	NODE NUMBER	RELAXATION FACTOR
1	62	0.4489E-01	17	0.290E-01	19	1.00
2	12	-0.3475E-01	17	0.341E-01	15	0.590
3	18	0.2838E-01	15	0.370E-01	15	0.361
4	12	0.2918E-01	15	0.221E-01	15	1.00
5	4	-0.9961E-02	3	0.105E-01	25	0.796
6	0	-0.9961E-02	3	0.905E-02	25	1.00

*** NODAL FLUID FLUX VALUES ***

NODAL FLUXES FOR FLUID PHASE # 1

NODE	FLUID FLUX	NODE	FLUID FLUX	NODE	FLUID FLUX	NODE	FLUID FLUX	NODE	FLUID FLUX
1	-3.3173E-05	2	-3.3173E-05	41	3.1709E-06	42	3.1709E-06		

SUM OF ABOVE FLUX VALUES = -6.00044E-05

NODAL FLUXES FOR FLUID PHASE # 2

NODE	FLUID FLUX	NODE	FLUID FLUX	NODE	FLUID FLUX	NODE	FLUID FLUX	NODE	FLUID FLUX
1	0.0000E+00	2	0.0000E+00	41	2.8538E-05	42	2.8538E-05		

SUM OF ABOVE FLUX VALUES = 5.70760E-05

COMPUTATIONAL TIME STEP VALUE = 0.4517E+06 CURRENT TIME = 0.8896E+07

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM HEAD ERROR	NODE NUMBER	MAXIMUM SATUR. ERROR	NODE NUMBER	RELAXATION FACTOR
1	38	0.8020E-01	15	0.492E-01	15	1.00
2	14	0.2664E-01	15	0.152E-01	13	1.00
3	10	-0.1993E-01	15	0.152E-01	13	0.601
4	0	-0.9443E-02	15	0.779E-02	29	1.00

*** NODAL FLUID FLUX VALUES ***

NODAL FLUXES FOR FLUID PHASE # 1

NODE	FLUID FLUX	NODE	FLUID FLUX	NODE	FLUID FLUX	NODE	FLUID FLUX	NODE	FLUID FLUX
1	-3.3163E-05	2	-3.3163E-05	41	3.1709E-06	42	3.1709E-06		

SUM OF ABOVE FLUX VALUES = -5.99846E-05

NODAL FLUXES FOR FLUID PHASE # 2

NODE	FLUID FLUX	NODE	FLUID FLUX	NODE	FLUID FLUX	NODE	FLUID FLUX	NODE	FLUID FLUX
1	0.0000E+00	2	0.0000E+00	41	2.8538E-05	42	2.8538E-05		

SUM OF ABOVE FLUX VALUES = 5.70760E-05

*** NODAL PRESSURE VALUES ***

NODE	PRESSURE (Pn)	NODE	PRESSURE (Pn)	NODE	PRESSURE (Pn)	NODE	PRESSURE (Pn)	NODE	PRESSURE (Pn)
1	1.50004E+05	2	1.50004E+05	3	1.47514E+05	4	1.47514E+05	5	1.45211E+05
6	1.45211E+05	7	1.42674E+05	8	1.42674E+05	9	1.40256E+05	10	1.40256E+05
11	1.37740E+05	12	1.37740E+05	13	1.35349E+05	14	1.35349E+05	15	1.34214E+05
16	1.34214E+05	17	1.32086E+05	18	1.32086E+05	19	1.29904E+05	20	1.29904E+05
21	1.27655E+05	22	1.27655E+05	23	1.25382E+05	24	1.25382E+05	25	1.23104E+05
26	1.23104E+05	27	1.20833E+05	28	1.20833E+05	29	1.18497E+05	30	1.18497E+05
31	1.16235E+05	32	1.16235E+05	33	1.13933E+05	34	1.13933E+05	35	1.11629E+05
36	1.11629E+05	37	1.09321E+05	38	1.09321E+05	39	1.07035E+05	40	1.07035E+05
41	1.06386E+05	42	1.06386E+05						

*** NODAL VALUES OF NAPL SATURATION ***

NODE	SATURAT. (Sn)	NODE	SATURAT. (Sn)	NODE	SATURAT. (Sn)	NODE	SATURAT. (Sn)	NODE	SATURAT. (Sn)
1	0.00000E+00	2	0.00000E+00	3	0.00000E+00	4	0.00000E+00	5	0.00000E+00
6	0.00000E+00	7	0.00000E+00	8	0.00000E+00	9	0.00000E+00	10	0.00000E+00
11	0.00000E+00	12	0.00000E+00	13	0.00000E+00	14	0.00000E+00	15	9.26367E-02
16	9.26367E-02	17	0.11033	18	0.11033	19	0.13989	20	0.13989
21	0.16221	22	0.16221	23	0.18161	24	0.18161	25	0.20563
26	0.20563	27	0.25849	28	0.25849	29	0.30238	30	0.30238
31	0.35434	32	0.35434	33	0.40052	34	0.40052	35	0.44598
36	0.44598	37	0.49843	38	0.49843	39	0.29726	40	0.29726
41	0.22722	42	0.22722						

*** NODAL VALUES OF WATER SATURATION ***

NODE	SATURAT. (Sw)	NODE	SATURAT. (Sw)	NODE	SATURAT. (Sw)	NODE	SATURAT. (Sw)	NODE	SATURAT. (Sw)
1	1.0000	2	1.0000	3	1.0000	4	1.0000	5	1.0000
6	1.0000	7	1.0000	8	1.0000	9	1.0000	10	1.0000
11	1.0000	12	1.0000	13	1.0000	14	1.0000	15	0.90736
16	0.90736	17	0.88967	18	0.88967	19	0.86011	20	0.86011
21	0.83779	22	0.83779	23	0.81839	24	0.81839	25	0.79437
26	0.79437	27	0.74153	28	0.74153	29	0.69763	30	0.69763
31	0.64676	32	0.64676	33	0.59997	34	0.59997	35	0.55418
36	0.55418	37	0.50933	38	0.50933	39	0.47099	40	0.47099
41	0.31136	42	0.31136						

*** FLUID FLOW MASS BALANCE INFORMATION AT TIME = 0.8896E+07***

*** MASS BALANCE, FLUID, AND FLOW INFORMATION ***

FLUID PHASE NUMBER	1
NET FLOW RATE DUE TO BOUNDARY FLUX AND SINKS	-5.99846E-05
RATE OF FLUID ACCUMULATION	-5.99846E-05
MASS BALANCE ERROR	-1.49864E-16
NORMALIZED MASS BALANCE ERROR	1.12975E-12
CUMULATIVE FLUID STORAGE	-5.28797E+02

*** MASS BALANCE, FLUID, AND FLOW INFORMATION ***

FLUID PHASE NUMBER	2
NET FLOW RATE DUE TO BOUNDARY FLUX AND SINKS	5.70760E-05
RATE OF FLUID ACCUMULATION	5.70760E-05
MASS BALANCE ERROR	-3.38813E-20
NORMALIZED MASS BALANCE ERROR	2.96809E-16
CUMULATIVE FLUID STORAGE	5.07771E+02

***** SAMFT2D HAS SOLVED THE PROBLEM *****

*** CPU TIME USED: 267.4 SECS. ***

- 6) Nonlinear iteration summary for each time step;
- 7) For each selected output time value:
 - nodal values of water pressure
 - nodal values of water and NAPL saturations
 - element saturation values and Darcy velocities
 - summary of mass balance information.
- 8) CPU time for the simulation.

10.6 SOLUTE TRANSPORT PROBLEM

10.6.1 Input Data

This problem is the two-dimensional transport problem described in Section 4.3.4. The main input data file on unit 5 is given in Table 10.9. An additional data file containing element velocities and water saturation is also required in the transport simulation. This file was created by the code from a prior flow simulation described in Section 4.2.4.

10.6.2 Output

Output for the transport simulation problem is listed in Table 10.10. The output file is organized as follows:

- 1) Summary of input control parameters;
- 2) Summary of the problem geometry and material properties;
- 3) Summary of prescribed boundary conditions;
- 4) Element velocities and saturation read from the file on unit 9;

Table 10.9. Input data file for the solute transport problem.

1	1																				GROUP 1	
		2-D TRANSPORT BENEATH A LANDFILL (N-R METHOD) BY SAMFT2D																			GROUP 2	
0	1	1	0	1	1	2	1	651	600	1	0	0									GROUP 3	
1	20		0.1		0.01		0.01		9.805		0.0	0	0								GROUP 4	
1	1	0	3	0	1	0	1	0	1	0	0	0									GROUP 5	
		0.0E00																			GROUP 7B	
		3.0E0		0.1E00		0.0E00		0.0E00		0.25E00		1.46E00									GROUP 10A	
		0.0E00																			GROUP 10B	
		0.0E00																			GROUP 10C	
21	31		5.0		1.75		0	0													GROUP 11	
		5.0		1.75		150.0		35.0		1.0		1.0		0.0		0.0					GROUP 13A	
26	31	0	0																		GROUP 14A	
1	1		0.0																			GROUP 14B
2	1		0.0																			GROUP 14B
3	1		0.0																			GROUP 14B
4	1		0.0																			GROUP 14B
5	1		0.0																			GROUP 14B
6	1		0.0																			GROUP 14B
7	1		0.0																			GROUP 14B
8	1		0.0																			GROUP 14B
9	1		0.0																			GROUP 14B
10	1		0.0																			GROUP 14B
11	1		0.0																			GROUP 14B
12	1		0.0																			GROUP 14B
13	1		0.0																			GROUP 14B
14	1		0.0																			GROUP 14B
15	1		0.0																			GROUP 14B
16	1		0.0																			GROUP 14B
17	1		0.0																			GROUP 14B
18	1		0.0																			GROUP 14B
19	1		0.0																			GROUP 14B
20	1		0.0																			GROUP 14B
21	1		0.0																			GROUP 14B
105	1		1.0																			GROUP 14B
126	1		1.0																			GROUP 14B
147	1		1.0																			GROUP 14B
168	1		1.0																			GROUP 14B
189	1		1.0																			GROUP 14B
21	1	0.0	7.927E-8																			GROUP 14C
42	1	0.0	1.585E-7																			-----
63	1	0.0	1.585E-7																			-----
84	1	0.0	1.585E-7																			-----
105	1	0.0	1.585E-7																			-----
126	1	0.0	1.585E-7																			-----
147	1	0.0	1.585E-7																			-----
168	1	0.0	1.585E-7																			-----
189	1	0.0	1.585E-7																			-----
210	1	0.0	1.585E-7																			-----
231	1	0.0	1.585E-7																			-----
252	1	0.0	1.585E-7																			-----
273	1	0.0	1.585E-7																			-----
294	1	0.0	1.585E-7																			-----
315	1	0.0	1.585E-7																			-----
336	1	0.0	1.585E-7																			-----
357	1	0.0	1.585E-7																			-----
378	1	0.0	1.585E-7																			-----
399	1	0.0	1.585E-7																			-----
420	1	0.0	1.585E-7																			-----
441	1	0.0	1.585E-7																			-----
462	1	0.0	1.585E-7																			-----
483	1	0.0	1.585E-7																			-----
504	1	0.0	1.585E-7																			-----
525	1	0.0	1.585E-7																			-----
546	1	0.0	1.585E-7																			-----

567	1	0.0	1.585E-7															-----
588	1	0.0	1.585E-7															-----
609	1	0.0	1.585E-7															-----
630	1	0.0	1.585E-7															-----
651	1	0.0	7.927E-8															-----
1		0.0	0.0															GROUP 18
1		0.2	0.0			0.0												GROUP 19
51																		GROUP 20A
1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16			GROUP 20B
17	18	19	20	21	42	63	84	105	126	147	168	189	210	231	252			GROUP 20B
273	294	315	336	357	378	399	420	441	462	483	504	525	546	567	588			GROUP 20B
609	630	651																GROUP 20B

Table 10.10. Output for the solute transport problem.

 THIS OUTPUT GENERATED BY SAMFT2D
 INPUT FILE NAME = 2D10-6.DAT

PROBLEM IDENTIFICATION NUMBER = 1
 PROBLEM EXECUTION INDEX.....(IEXEC) = 1

PROBLEM TITLE

 2-D TRANSPORT BENEATH A LANDFILL (N-R METHOD) BY SAMFT2D

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) = 1
 NUMBER OF ACTIVE FLUID PHASES..... (NMPHAS) = 1
 MATERIAL NUMBER INPUT ? (1=YES,0=NO)(IMNUMR).... = 0
 TOTAL NUMBER OF DEPENDENT VARIABLES.....(NVAR) = 1
 STEADY STATE SIMULATION(1=YES, 0=NO).....(ISSTA) = 1
 TIME STEP GENERATION INDEX (1=YES, 0=NO) ..(ITSGN) = 2
 NUMBER OF TIME STEPS(NTS) = 1
 TOTAL NUMBER OF NODES(NP) = 651
 TOTAL NUMBER OF ELEMENTS(NE) = 600
 NUMBER OF POROUS MATERIALS(NMAT) = 1
 SOIL CONSTITUTIVE DATA(0=FUNCTION,1=TABLE)(KPROP) = 0
 INITIAL CONDITION NON-UNIFORMITY INDEX(NONU) = 0
 SEQUENCE OF NODE NUMBERING (0=Y-,1=X-DIR).(ISWAP) = 0

INPUT / OUTPUT CONTROL PARAMETERS

 VELOCITY/INPUT.....(NVREAD) = 1
 BOUNDARY NODE DATA READ (1=YES, 0=NO)....(IOUTLT) = 1
 NUMBER OF NODES FOR WHICH I.C. ARE READ....(NPIN) = 0
 OUTPUT REQUIREMENT INDICATOR:
 (0=ALL DATA, 1=NO ELEMENT DATA,
 2=NO MESH DATA, 3=NO MESH AND I.C. DATA..(IPRD) = 3
 UNIT 9 OUTPUT (1=YES, 0=NO).....(NVWRIT) = 0
 VELOCITY PRINTOUT CONTROL INDEX.....(NVPR) = 1
 UNIT 10 OUTPUT (0=NONE, N=NTH).....(NPLOT) = 0
 NODAL VALUE PRINTOUT CONTROL INDEX.....(NSTEP) = 1
 OBSERVATION NODE INDEX.....(IOBSND) = 0
 MASS BALANCE TO BE PERFORMED (1=YES,0=NO).(IMBAL) = 1
 UNIT 8 OUTPUT (1=YES, 0=NO).....(NOWRIT) = 0
 PRINT CHECK OPTION INDEX.....(IPRCHK) = 0
 PRESSURE HEAD OUTPUT OPTION INDEX.....(IPWOUT) = 0
 OUTPUT SPECIFIED TIME INDEX.....(NPRCON) = 0

TIME STEP. PARAMETER FOR TRANSPORT SIMULATION.(IKALL) = 1

CONC. TOLERANCE FOR TRANSPORT MATRIX SOLTN..(CTOL) = 0.1000E-01

DEFAULT INITIAL CONDITION FOR TRANSPORT PROBLEM

PRESCRIBED INITIAL CONCENTRATION VALUE....(CIDFAL) = 0.0000E+00

TRANSPORT PROPERTIES OF POROUS MEDIA

MATERIAL NUMBER: 1 (I)

LONGITUDINAL DISPERSIVITY.....(PROPJ(I,1)) = 0.3000E+01
TRANSVERSE DISPERSIVITY.....(PROPJ(I,2)) = 0.1000E+00
TORTUOSITY FACTOR.....(PROPJ(I,3)) = 0.0000E+00
DIFFUSION COEFFICIENT PARAMETER.....(PROPJ(I,4)) = 0.0000E+00
EFFECTIVE POROSITY.....(PROPJ(I,5)) = 0.2500E+00
BULK DENSITY (g/cm**3)(PROPJ(I,6)) = 0.1460E+01

MOLECULAR DIFFUSION COEFFICIENT OF PHASE 1 THROUGH NTPHAS

0.0000E+00

SOLUTE PROPERTIES

MATERIAL NUMBER: 1 (I)

DECAY COEFFICIENT (RPROP(I,1)) = 0.0000E+00
DISTRIBUTION COEFFICIENT (RPROP(I,2)) = 0.0000E+00

GRID SPECIFICATION DATA

NUMBER OF ROWS.....(NROWS) = 21
NUMBER OF COLUMNS.....(NCOLS) = 31
MAXIMUM ALLOWABLE X-SPACING.....(DXMAX) = 5.00
MAXIMUM ALLOWABLE Y-SPACING.....(DYMAX) = 1.75
INPUT INDICATOR FOR GRIDLINE COORD.....(IXYZRD) = 0
HORIZONTAL PLANE DOMAIN INDICATOR.....(IHORGR) = 0

X-INCREMENT OF THE FIRST GRID BLOCK(DX) = 5.000
Y-INCREMENT OF THE FIRST GRID BLOCK(DY) = 1.750
MAXIMUM VALUE OF X-COORDINATE(XO) = 150.000
MAXIMUM VALUE OF Y-COORDINATE(YO) = 35.000
X-INCREMENT MULTIPLIER(SCFX) = 1.000
Y-INCREMENT MULTIPLIER(SCFY) = 1.000
MINIMUM VALUE OF X-COORDINATE(XSTART) = 0.000
MINIMUM VALUE OF Y-COORDINATE(YSTART) = 0.000

BOUNDARY CONDITION DATA

NUMBER OF STEADY DIRICHLET BOUNDARIES (NBTO) = 26
NUMBER OF STEADY FLUX BOUNDARIES (NDFLUX) = 31
NUMBER OF TRANSIENT DIRICHLET BOUNDARIES.... (NBHVAR) = 0
NUMBER OF TRANSIENT FLUX BOUNDARIES.... (NBFVAR) = 0

STEADY-STATE DIRICHLET BOUNDARY CONDITIONS

INDEX	NODE NO.	D.V. NO.	PRESCRIBED VALUE	B.C. IDENTIFIER
-------	----------	----------	------------------	-----------------

1	1	1	0.000000E+00	0
2	2	1	0.000000E+00	0
3	3	1	0.000000E+00	0
4	4	1	0.000000E+00	0
5	5	1	0.000000E+00	0
6	6	1	0.000000E+00	0
7	7	1	0.000000E+00	0
8	8	1	0.000000E+00	0
9	9	1	0.000000E+00	0
10	10	1	0.000000E+00	0
11	11	1	0.000000E+00	0
12	12	1	0.000000E+00	0
13	13	1	0.000000E+00	0
14	14	1	0.000000E+00	0
15	15	1	0.000000E+00	0
16	16	1	0.000000E+00	0
17	17	1	0.000000E+00	0
18	18	1	0.000000E+00	0
19	19	1	0.000000E+00	0
20	20	1	0.000000E+00	0
21	21	1	0.000000E+00	0
22	105	1	1.00000	0
23	126	1	1.00000	0
24	147	1	1.00000	0
25	168	1	1.00000	0
26	189	1	1.00000	0

STEADY-STATE FLUX BOUNDARY CONDITIONS

INDEX	NODE NO.	D.V. NO.	SOLUTE FLUX	FLUID FLUX VALUE
1	21	1	0.000000E+00	7.927000E-08
2	42	1	0.000000E+00	1.585000E-07
3	63	1	0.000000E+00	1.585000E-07
4	84	1	0.000000E+00	1.585000E-07
5	105	1	0.000000E+00	1.585000E-07
6	126	1	0.000000E+00	1.585000E-07
7	147	1	0.000000E+00	1.585000E-07
8	168	1	0.000000E+00	1.585000E-07
9	189	1	0.000000E+00	1.585000E-07
10	210	1	0.000000E+00	1.585000E-07
11	231	1	0.000000E+00	1.585000E-07
12	252	1	0.000000E+00	1.585000E-07
13	273	1	0.000000E+00	1.585000E-07
14	294	1	0.000000E+00	1.585000E-07
15	315	1	0.000000E+00	1.585000E-07
16	336	1	0.000000E+00	1.585000E-07
17	357	1	0.000000E+00	1.585000E-07
18	378	1	0.000000E+00	1.585000E-07
19	399	1	0.000000E+00	1.585000E-07
20	420	1	0.000000E+00	1.585000E-07
21	441	1	0.000000E+00	1.585000E-07
22	462	1	0.000000E+00	1.585000E-07
23	483	1	0.000000E+00	1.585000E-07
24	504	1	0.000000E+00	1.585000E-07
25	525	1	0.000000E+00	1.585000E-07
26	546	1	0.000000E+00	1.585000E-07
27	567	1	0.000000E+00	1.585000E-07
28	588	1	0.000000E+00	1.585000E-07
29	609	1	0.000000E+00	1.585000E-07
30	630	1	0.000000E+00	1.585000E-07
31	651	1	0.000000E+00	7.927000E-08

TRANSPORT SIMULATION CONTROL DATA

STEADY-STATE VELOCITY FIELD (0=NO,1=YES)..(IVSTED) = 1
 UPSTREAM FACTOR IN X-DIRECTION.....(WFAC) = 0.00E+00
 UPSTREAM FACTOR IN Y-DIRECTION.....(YFAC) = 0.00E+00

DEFAULT PHASE SATURATION AND DARCY VELOCITY VALUES

FLUID PHASE NUMBER 1

PHASE SATURATION (DEFAULT VALUE)..... = 0.2000E+00
 X-COMPONENT OF DARCY VELOCITY (DEFAULT VALUE)..... = 0.0000E+00
 Y-COMPONENT OF DARCY VELOCITY (DEFAULT VALUE)..... = 0.0000E+00

LIST OF BOUNDARY NODE NUMBERS

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
17	18	19	20	21	42	63	84	105	126	147	168	189	210	231	252
273	294	315	336	357	378	399	420	441	462	483	504	525	546	567	588
609	630	651													

MATRIX BANDWIDTH REQUIRED IN THIS SIMULATION= 45----

 *** RESULT OF STEADY-STATE ANALYSIS ***

*** ELEMENTAL FLUID VELOCITY FROM TAPE 9 ***

ELEMENT	X-VELOCITY	Y-VELOCITY	ELEMENT	X-VELOCITY	Y-VELOCITY	ELEMENT	X-VELOCITY	Y-VELOCITY
-----	-----	-----	-----	-----	-----	-----	-----	-----
1	2.179E-07	-3.067E-11	2	2.175E-07	-3.771E-10	3	2.168E-07	-7.744E-10
4	2.162E-07	-1.710E-09	5	2.153E-07	-1.566E-09	6	2.138E-07	-1.974E-09
7	2.120E-07	-2.460E-09	8	2.102E-07	-3.504E-09	9	2.080E-07	-3.469E-09
10	2.051E-07	-3.934E-09	11	2.020E-07	-4.286E-09	12	1.991E-07	-4.625E-09
13	1.378E-07	2.495E-08	14	4.924E-08	-2.707E-08	15	1.085E-08	-6.679E-08
16	2.207E-09	-6.926E-08	17	4.984E-10	-5.784E-08	18	1.374E-10	-4.626E-08
19	4.774E-11	-3.898E-08	20	2.172E-11	-3.521E-08	21	2.197E-07	-5.369E-10
22	2.195E-07	-1.567E-09	23	2.191E-07	-2.646E-09	24	2.184E-07	-3.638E-09
25	2.175E-07	-4.912E-09	26	2.163E-07	-6.138E-09	27	2.149E-07	-7.494E-09
28	2.131E-07	-8.853E-09	29	2.109E-07	-1.060E-08	30	2.083E-07	-1.244E-08
31	2.048E-07	-1.458E-08	32	1.997E-07	-1.701E-08	33	1.593E-07	-3.734E-08
34	7.812E-08	-5.805E-08	35	2.197E-08	-7.300E-08	36	5.036E-09	-7.009E-08
37	1.208E-09	-5.781E-08	38	3.431E-10	-4.616E-08	39	1.183E-10	-3.891E-08
40	4.670E-11	-3.517E-08	41	2.235E-07	-7.922E-10	42	2.234E-07	-2.395E-09
43	2.230E-07	-4.018E-09	44	2.225E-07	-5.723E-09	45	2.218E-07	-7.458E-09
46	2.210E-07	-9.327E-09	47	2.199E-07	-1.132E-08	48	2.188E-07	-1.354E-08
49	2.174E-07	-1.596E-08	50	2.160E-07	-1.876E-08	51	2.146E-07	-2.209E-08
52	2.136E-07	-2.631E-08	53	1.693E-07	-3.769E-08	54	8.246E-08	-6.415E-08
55	2.428E-08	-7.590E-08	56	5.914E-09	-7.051E-08	57	1.489E-09	-5.764E-08
58	4.368E-10	-4.599E-08	59	1.536E-10	-3.881E-08	60	6.230E-11	-3.512E-08
61	2.287E-07	-9.994E-10	62	2.286E-07	-3.003E-09	63	2.284E-07	-5.038E-09
64	2.280E-07	-7.112E-09	65	2.276E-07	-9.263E-09	66	2.271E-07	-1.149E-08
67	2.265E-07	-1.384E-08	68	2.258E-07	-1.632E-08	69	2.251E-07	-1.896E-08
70	2.245E-07	-2.177E-08	71	2.239E-07	-2.471E-08	72	2.229E-07	-2.769E-08

73	1.759E-07	-4.118E-08	74	8.469E-08	-6.566E-08	75	2.482E-08	-7.644E-08
76	6.104E-09	-7.042E-08	77	1.564E-09	-5.735E-08	78	4.670E-10	-4.576E-08
79	1.666E-10	-3.869E-08	80	6.783E-11	-3.506E-08	81	2.348E-07	-1.130E-09
82	2.347E-07	-3.397E-09	83	2.346E-07	-5.682E-09	84	2.344E-07	-8.000E-09
85	2.342E-07	-1.036E-08	86	2.339E-07	-1.278E-08	87	2.335E-07	-1.526E-08
88	2.332E-07	-1.782E-08	89	2.328E-07	-2.044E-08	90	2.324E-07	-2.315E-08
91	2.321E-07	-2.592E-08	92	2.311E-07	-2.889E-08	93	1.808E-07	-4.238E-08
94	8.565E-08	-6.678E-08	95	2.493E-08	-7.665E-08	96	6.140E-09	-7.016E-08
97	1.582E-09	-5.700E-08	98	4.762E-10	-4.551E-08	99	1.709E-10	-3.855E-08
100	6.994E-11	-3.499E-08	101	2.415E-07	-1.210E-09	102	2.415E-07	-3.632E-09
103	2.414E-07	-6.066E-09	104	2.413E-07	-8.518E-09	105	2.411E-07	-1.100E-08
106	2.410E-07	-1.350E-08	107	2.408E-07	-1.605E-08	108	2.406E-07	-1.863E-08
109	2.404E-07	-2.124E-08	110	2.402E-07	-2.390E-08	111	2.400E-07	-2.659E-08
112	2.386E-07	-2.944E-08	113	1.848E-07	-4.353E-08	114	8.607E-08	-6.757E-08
115	2.485E-08	-7.674E-08	116	6.117E-09	-6.985E-08	117	1.583E-09	-5.663E-08
118	4.791E-10	-4.526E-08	119	1.729E-10	-3.841E-08	120	7.094E-11	-3.492E-08
121	2.486E-07	-1.257E-09	122	2.486E-07	-3.771E-09	123	2.485E-07	-6.291E-09
124	2.484E-07	-8.821E-09	125	2.483E-07	-1.137E-08	126	2.482E-07	-1.392E-08
127	2.481E-07	-1.650E-08	128	2.480E-07	-1.910E-08	129	2.479E-07	-2.172E-08
130	2.478E-07	-2.435E-08	131	2.476E-07	-2.700E-08	132	2.457E-07	-2.988E-08
133	1.883E-07	-4.452E-08	134	8.613E-08	-6.829E-08	135	2.465E-08	-7.678E-08
136	6.065E-09	-6.952E-08	137	1.575E-09	-5.625E-08	138	4.795E-10	-4.499E-08
139	1.738E-10	-3.827E-08	140	7.155E-11	-3.485E-08	141	2.558E-07	-1.285E-09
142	2.558E-07	-3.855E-09	143	2.558E-07	-6.429E-09	144	2.558E-07	-9.007E-09
145	2.557E-07	-1.159E-08	146	2.556E-07	-1.419E-08	147	2.556E-07	-1.679E-08
148	2.555E-07	-1.940E-08	149	2.554E-07	-2.202E-08	150	2.553E-07	-2.466E-08
151	2.552E-07	-2.729E-08	152	2.526E-07	-3.024E-08	153	1.913E-07	-4.549E-08
154	8.594E-08	-6.896E-08	155	2.438E-08	-7.679E-08	156	5.995E-09	-6.917E-08
157	1.563E-09	-5.585E-08	158	4.784E-10	-4.473E-08	159	1.743E-10	-3.813E-08
160	7.194E-11	-3.478E-08	161	2.632E-07	-1.304E-09	162	2.632E-07	-3.911E-09
163	2.632E-07	-6.520E-09	164	2.632E-07	-9.132E-09	165	2.631E-07	-1.175E-08
166	2.631E-07	-1.437E-08	167	2.630E-07	-1.699E-08	168	2.630E-07	-1.962E-08
169	2.629E-07	-2.225E-08	170	2.628E-07	-2.489E-08	171	2.628E-07	-2.753E-08
172	2.592E-07	-3.058E-08	173	1.940E-07	-4.646E-08	174	8.553E-08	-6.962E-08
175	2.405E-08	-7.677E-08	176	5.911E-09	-6.880E-08	177	1.547E-09	-5.545E-08
178	4.763E-10	-4.446E-08	179	1.744E-10	-3.799E-08	180	7.218E-11	-3.471E-08
181	2.707E-07	-1.318E-09	182	2.707E-07	-3.953E-09	183	2.707E-07	-6.589E-09
184	2.707E-07	-9.226E-09	185	2.706E-07	-1.186E-08	186	2.706E-07	-1.451E-08
187	2.706E-07	-1.715E-08	188	2.705E-07	-1.979E-08	189	2.704E-07	-2.244E-08
190	2.704E-07	-2.509E-08	191	2.703E-07	-2.774E-08	192	2.656E-07	-3.093E-08
193	1.964E-07	-4.746E-08	194	8.493E-08	-7.026E-08	195	2.368E-08	-7.673E-08
196	5.817E-09	-6.841E-08	197	1.529E-09	-5.503E-08	198	4.734E-10	-4.418E-08
199	1.741E-10	-3.784E-08	200	7.230E-11	-3.464E-08	201	2.783E-07	-1.329E-09
202	2.783E-07	-3.987E-09	203	2.783E-07	-6.645E-09	204	2.782E-07	-9.304E-09
205	2.782E-07	-1.196E-08	206	2.782E-07	-1.462E-08	207	2.781E-07	-1.729E-08
208	2.781E-07	-1.995E-08	209	2.780E-07	-2.261E-08	210	2.780E-07	-2.528E-08
211	2.779E-07	-2.794E-08	212	2.719E-07	-3.128E-08	213	1.984E-07	-4.848E-08
214	8.415E-08	-7.089E-08	215	2.326E-08	-7.668E-08	216	5.713E-09	-6.800E-08
217	1.508E-09	-5.461E-08	218	4.698E-10	-4.391E-08	219	1.737E-10	-3.770E-08
220	7.232E-11	-3.457E-08	221	2.859E-07	-1.340E-09	222	2.859E-07	-4.017E-09
223	2.859E-07	-6.695E-09	224	2.859E-07	-9.374E-09	225	2.858E-07	-1.205E-08
226	2.858E-07	-1.473E-08	227	2.858E-07	-1.741E-08	228	2.857E-07	-2.009E-08
229	2.857E-07	-2.277E-08	230	2.856E-07	-2.545E-08	231	2.856E-07	-2.814E-08
232	2.780E-07	-3.166E-08	233	2.001E-07	-4.953E-08	234	8.320E-08	-7.151E-08
235	2.280E-08	-7.660E-08	236	5.601E-09	-6.758E-08	237	1.485E-09	-5.418E-08
238	4.656E-10	-4.363E-08	239	1.730E-10	-3.755E-08	240	7.225E-11	-3.450E-08
241	2.936E-07	-1.349E-09	242	2.936E-07	-4.046E-09	243	2.936E-07	-6.743E-09
244	2.936E-07	-9.441E-09	245	2.935E-07	-1.214E-08	246	2.935E-07	-1.484E-08
247	2.935E-07	-1.753E-08	248	2.934E-07	-2.023E-08	249	2.934E-07	-2.293E-08
250	2.933E-07	-2.563E-08	251	2.932E-07	-2.832E-08	252	2.838E-07	-3.207E-08
253	2.014E-07	-5.061E-08	254	8.208E-08	-7.212E-08	255	2.231E-08	-7.650E-08
256	5.481E-09	-6.714E-08	257	1.460E-09	-5.374E-08	258	4.607E-10	-4.335E-08
259	1.720E-10	-3.741E-08	260	7.208E-11	-3.443E-08	261	3.013E-07	-1.359E-09
262	3.013E-07	-4.075E-09	263	3.013E-07	-6.791E-09	264	3.013E-07	-9.507E-09
265	3.013E-07	-1.222E-08	266	3.012E-07	-1.494E-08	267	3.012E-07	-1.765E-08
268	3.011E-07	-2.037E-08	269	3.011E-07	-2.308E-08	270	3.010E-07	-2.580E-08
271	3.010E-07	-2.851E-08	272	2.895E-07	-3.250E-08	273	2.023E-07	-5.172E-08
274	8.081E-08	-7.271E-08	275	2.178E-08	-7.637E-08	276	5.355E-09	-6.668E-08
277	1.434E-09	-5.330E-08	278	4.553E-10	-4.306E-08	279	1.709E-10	-3.726E-08

280	7.182E-11	-3.436E-08	281	3.091E-07	-1.369E-09	282	3.091E-07	-4.104E-09
283	3.091E-07	-6.840E-09	284	3.091E-07	-9.575E-09	285	3.090E-07	-1.231E-08
286	3.090E-07	-1.504E-08	287	3.090E-07	-1.778E-08	288	3.089E-07	-2.051E-08
289	3.089E-07	-2.324E-08	290	3.088E-07	-2.597E-08	291	3.087E-07	-2.870E-08
292	2.949E-07	-3.296E-08	293	2.028E-07	-5.286E-08	294	7.940E-08	-7.328E-08
295	2.123E-08	-7.622E-08	296	5.222E-09	-6.621E-08	297	1.406E-09	-5.284E-08
298	4.494E-10	-4.278E-08	299	1.696E-10	-3.711E-08	300	7.148E-11	-3.429E-08
301	3.170E-07	-1.379E-09	302	3.170E-07	-4.136E-09	303	3.169E-07	-6.892E-09
304	3.169E-07	-9.647E-09	305	3.169E-07	-1.240E-08	306	3.168E-07	-1.515E-08
307	3.168E-07	-1.791E-08	308	3.168E-07	-2.066E-08	309	3.167E-07	-2.340E-08
310	3.166E-07	-2.615E-08	311	3.166E-07	-2.889E-08	312	3.000E-07	-3.346E-08
313	2.029E-07	-5.403E-08	314	7.783E-08	-7.383E-08	315	2.065E-08	-7.605E-08
316	5.085E-09	-6.572E-08	317	1.377E-09	-5.238E-08	318	4.430E-10	-4.249E-08
319	1.680E-10	-3.697E-08	320	7.105E-11	-3.422E-08	321	3.249E-07	-1.391E-09
322	3.249E-07	-4.170E-09	323	3.248E-07	-6.949E-09	324	3.248E-07	-9.728E-09
325	3.248E-07	-1.250E-08	326	3.247E-07	-1.528E-08	327	3.247E-07	-1.805E-08
328	3.246E-07	-2.082E-08	329	3.246E-07	-2.359E-08	330	3.245E-07	-2.635E-08
331	3.244E-07	-2.910E-08	332	3.048E-07	-3.401E-08	333	2.026E-07	-5.522E-08
334	7.614E-08	-7.436E-08	335	2.005E-08	-7.585E-08	336	4.943E-09	-6.521E-08
337	1.346E-09	-5.192E-08	338	4.362E-10	-4.221E-08	339	1.663E-10	-3.638E-08
340	7.055E-11	-3.415E-08	341	3.328E-07	-1.404E-09	342	3.328E-07	-4.209E-09
343	3.328E-07	-7.015E-09	344	3.328E-07	-9.819E-09	345	3.327E-07	-1.262E-08
346	3.327E-07	-1.542E-08	347	3.326E-07	-1.822E-08	348	3.326E-07	-2.102E-08
349	3.325E-07	-2.381E-08	350	3.324E-07	-2.659E-08	351	3.323E-07	-2.938E-08
352	3.093E-07	-3.463E-08	353	2.018E-07	-5.642E-08	354	7.432E-08	-7.486E-08
355	1.943E-08	-7.562E-08	356	4.798E-09	-6.468E-08	357	1.314E-09	-5.145E-08
358	4.290E-10	-4.192E-08	359	1.644E-10	-3.667E-08	360	6.997E-11	-3.408E-08
361	3.409E-07	-1.418E-09	362	3.409E-07	-4.254E-09	363	3.409E-07	-7.088E-09
364	3.408E-07	-9.922E-09	365	3.408E-07	-1.275E-08	366	3.407E-07	-1.558E-08
367	3.407E-07	-1.841E-08	368	3.406E-07	-2.124E-08	369	3.405E-07	-2.406E-08
370	3.404E-07	-2.688E-08	371	3.403E-07	-2.970E-08	372	3.135E-07	-3.532E-08
373	2.007E-07	-5.762E-08	374	7.240E-08	-7.533E-08	375	1.880E-08	-7.537E-08
376	4.650E-09	-6.414E-08	377	1.282E-09	-5.097E-08	378	4.215E-10	-4.164E-08
379	1.624E-10	-3.653E-08	380	6.932E-11	-3.401E-08	381	3.491E-07	-1.435E-09
382	3.490E-07	-4.304E-09	383	3.490E-07	-7.171E-09	384	3.490E-07	-1.004E-08
385	3.489E-07	-1.290E-08	386	3.489E-07	-1.576E-08	387	3.488E-07	-1.638E-08
388	3.487E-07	-2.148E-08	389	3.486E-07	-2.434E-08	390	3.485E-07	-2.719E-08
391	3.484E-07	-3.004E-08	392	3.175E-07	-3.607E-08	393	1.991E-07	-5.885E-08
394	7.039E-08	-7.577E-08	395	1.816E-08	-7.508E-08	396	4.500E-09	-6.358E-08
397	1.249E-09	-5.050E-08	398	4.136E-10	-4.135E-08	399	1.603E-10	-3.638E-08
400	6.861E-11	-3.394E-08	401	3.573E-07	-1.454E-09	402	3.573E-07	-4.360E-09
403	3.573E-07	-7.265E-09	404	3.572E-07	-1.017E-08	405	3.572E-07	-1.307E-08
406	3.571E-07	-1.597E-08	407	3.570E-07	-1.886E-08	408	3.569E-07	-2.175E-08
409	3.568E-07	-2.464E-08	410	3.567E-07	-2.752E-08	411	3.566E-07	-3.040E-08
412	3.212E-07	-3.689E-08	413	1.972E-07	-6.009E-08	414	6.829E-08	-7.618E-08
415	1.751E-08	-7.477E-08	416	4.349E-09	-6.301E-08	417	1.215E-09	-5.001E-08
418	4.055E-10	-4.107E-08	419	1.580E-10	-3.624E-08	420	6.785E-11	-3.387E-08
421	3.657E-07	-1.476E-09	422	3.657E-07	-4.427E-09	423	3.656E-07	-7.375E-09
424	3.656E-07	-1.032E-08	425	3.655E-07	-1.326E-08	426	3.654E-07	-1.620E-08
427	3.653E-07	-1.913E-08	428	3.652E-07	-2.205E-08	429	3.651E-07	-2.497E-08
430	3.650E-07	-2.788E-08	431	3.648E-07	-3.079E-08	432	3.246E-07	-3.778E-08
433	1.948E-07	-6.134E-08	434	6.612E-08	-7.656E-08	435	1.685E-08	-7.443E-08
436	4.197E-09	-6.242E-08	437	1.181E-09	-4.953E-08	438	3.972E-10	-4.079E-08
439	1.556E-10	-3.610E-08	440	6.704E-11	-3.380E-08	441	3.742E-07	-1.505E-09
442	3.742E-07	-4.511E-09	443	3.741E-07	-7.514E-09	444	3.740E-07	-1.051E-08
445	3.740E-07	-1.350E-08	446	3.739E-07	-1.648E-08	447	3.737E-07	-1.945E-08
448	3.736E-07	-2.241E-08	449	3.735E-07	-2.535E-08	450	3.733E-07	-2.829E-08
451	3.732E-07	-3.122E-08	452	3.277E-07	-3.878E-08	453	1.920E-07	-6.260E-08
454	6.388E-08	-7.690E-08	455	1.619E-08	-7.406E-08	456	4.044E-09	-6.181E-08
457	1.146E-09	-4.904E-08	458	3.886E-10	-4.051E-08	459	1.530E-10	-3.596E-08
460	6.614E-11	-3.373E-08	461	3.829E-07	-1.544E-09	462	3.828E-07	-4.628E-09
463	3.828E-07	-7.705E-09	464	3.827E-07	-1.077E-08	465	3.826E-07	-1.382E-08
466	3.824E-07	-1.685E-08	467	3.823E-07	-1.986E-08	468	3.821E-07	-2.286E-08
469	3.819E-07	-2.583E-08	470	3.817E-07	-2.876E-08	471	3.815E-07	-3.172E-08
472	3.304E-07	-3.987E-08	473	1.887E-07	-6.388E-08	474	6.157E-08	-7.721E-08
475	1.552E-08	-7.366E-08	476	3.891E-09	-6.119E-08	477	1.111E-09	-4.855E-08
478	3.796E-10	-4.023E-08	479	1.503E-10	-3.582E-08	480	6.498E-11	-3.366E-08
481	3.918E-07	-1.603E-09	482	3.918E-07	-4.805E-09	483	3.917E-07	-7.994E-09
484	3.916E-07	-1.116E-08	485	3.914E-07	-1.430E-08	486	3.911E-07	-1.741E-08

487	3.909E-07	-2.048E-08	488	3.906E-07	-2.350E-08	489	3.904E-07	-2.646E-08
490	3.901E-07	-2.945E-08	491	3.898E-07	-3.225E-08	492	3.326E-07	-4.118E-08
493	1.850E-07	-6.520E-08	494	5.918E-08	-7.751E-08	495	1.485E-08	-7.324E-08
496	3.735E-09	-6.056E-08	497	1.075E-09	-4.806E-08	498	3.701E-10	-3.995E-08
499	1.473E-10	-3.568E-08	500	6.351E-11	-3.360E-08	501	4.012E-07	-1.694E-09
502	4.012E-07	-5.077E-09	503	4.010E-07	-8.444E-09	504	4.008E-07	-1.179E-08
505	4.005E-07	-1.508E-08	506	4.001E-07	-1.832E-08	507	3.997E-07	-2.148E-08
508	3.992E-07	-2.458E-08	509	3.987E-07	-2.758E-08	510	3.984E-07	-3.021E-08
511	3.979E-07	-3.342E-08	512	3.342E-07	-4.262E-08	513	1.807E-07	-6.666E-08
514	5.669E-08	-7.783E-08	515	1.415E-08	-7.281E-08	516	3.571E-09	-5.992E-08
517	1.036E-09	-4.758E-08	518	3.591E-10	-3.968E-08	519	1.436E-10	-3.555E-08
520	6.170E-11	-3.354E-08	521	4.112E-07	-1.803E-09	522	4.112E-07	-5.413E-09
523	4.110E-07	-9.045E-09	524	4.107E-07	-1.268E-08	525	4.102E-07	-1.633E-08
526	4.096E-07	-1.989E-08	527	4.088E-07	-2.329E-08	528	4.080E-07	-2.644E-08
529	4.072E-07	-2.945E-08	530	4.059E-07	-3.318E-08	531	4.052E-07	-3.371E-08
532	3.349E-07	-4.549E-08	533	1.753E-07	-6.861E-08	534	5.393E-08	-7.827E-08
535	1.338E-08	-7.242E-08	536	3.380E-09	-5.930E-08	537	9.847E-10	-4.710E-08
538	3.430E-10	-3.941E-08	539	1.375E-10	-3.541E-08	540	5.898E-11	-3.349E-08
541	4.217E-07	-1.807E-09	542	4.217E-07	-5.475E-09	543	4.218E-07	-9.265E-09
544	4.218E-07	-1.330E-08	545	4.216E-07	-1.757E-08	546	4.210E-07	-2.215E-08
547	4.197E-07	-2.689E-08	548	4.175E-07	-3.139E-08	549	4.149E-07	-3.442E-08
550	4.144E-07	-3.336E-08	551	4.113E-07	-4.427E-08	552	3.316E-07	-4.830E-08
553	1.683E-07	-7.172E-08	554	5.041E-08	-7.979E-08	555	1.228E-08	-7.236E-08
556	3.068E-09	-5.876E-08	557	8.895E-10	-4.666E-08	558	3.092E-10	-3.917E-08
559	1.238E-10	-3.529E-08	560	5.277E-11	-3.344E-08	561	4.313E-07	-1.480E-09
562	4.317E-07	-4.466E-09	563	4.325E-07	-7.723E-09	564	4.338E-07	-1.130E-08
565	4.353E-07	-1.582E-08	566	4.368E-07	-2.131E-08	567	4.378E-07	-2.849E-08
568	4.371E-07	-3.804E-08	569	4.315E-07	-5.150E-08	570	4.131E-07	-7.002E-08
571	4.088E-07	-2.784E-08	572	3.280E-07	-6.934E-08	573	1.527E-07	-9.073E-08
574	4.219E-08	-8.568E-08	575	9.737E-09	-7.310E-08	576	2.358E-09	-5.842E-08
577	6.716E-10	-4.632E-08	578	2.306E-10	-3.897E-08	579	9.143E-11	-3.519E-08
580	3.964E-11	-3.339E-08	581	4.373E-07	-4.283E-10	582	4.382E-07	-1.610E-09
583	4.401E-07	-2.971E-09	584	4.427E-07	-5.119E-09	585	4.465E-07	-6.622E-09
586	4.524E-07	-9.432E-09	587	4.607E-07	-1.367E-08	588	4.726E-07	-2.097E-08
589	4.910E-07	-3.218E-08	590	5.215E-07	-5.440E-08	591	4.336E-07	-3.025E-07
592	2.206E-07	-1.992E-07	593	7.818E-08	-1.349E-07	594	1.867E-08	-9.448E-08
595	4.011E-09	-7.421E-08	596	9.365E-10	-5.829E-08	597	2.612E-10	-4.612E-08
598	8.795E-11	-3.886E-08	599	3.330E-11	-3.514E-08	600	1.142E-11	-3.338E-08

ELEMENT SATURATION VALUES FROM TAPE 9

ELEMENT	WATER SAT.	ELEMENT	WATER SAT.	ELEMENT	WATER SAT.	ELEMENT	WATER SAT.	ELEMENT	WATER SAT.
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	0.9581	14	0.8339	15	0.6799
16	0.5600	17	0.4833	18	0.4393	19	0.4160	20	0.4043
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	0.9999	33	0.9565	34	0.8310	35	0.6776
36	0.5586	37	0.4825	38	0.4389	39	0.4158	40	0.4042
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	0.9998	53	0.9546	54	0.8272	55	0.6743
56	0.5564	57	0.4813	58	0.4382	59	0.4154	60	0.4040
61	1.000	62	1.000	63	1.000	64	1.000	65	1.000
66	1.000	67	1.000	68	1.000	69	1.000	70	1.000
71	1.000	72	0.9996	73	0.9524	74	0.8231	75	0.6707
76	0.5540	77	0.4798	78	0.4374	79	0.4151	80	0.4038
81	1.000	82	1.000	83	1.000	84	1.000	85	1.000
86	1.000	87	1.000	88	1.000	89	1.000	90	1.000
91	1.000	92	0.9994	93	0.9501	94	0.8189	95	0.6669
96	0.5515	97	0.4783	98	0.4366	99	0.4146	100	0.4036
101	1.000	102	1.000	103	1.000	104	1.000	105	1.000
106	1.000	107	1.000	108	1.000	109	1.000	110	1.000
111	1.000	112	0.9991	113	0.9476	114	0.8144	115	0.6630

116	0.5488	117	0.4768	118	0.4358	119	0.4142	120	0.4034
121	1.000	122	1.000	123	1.000	124	1.000	125	1.000
126	1.000	127	1.000	128	1.000	129	1.000	130	1.000
131	1.000	132	0.9986	133	0.9449	134	0.8098	135	0.6590
136	0.5462	137	0.4752	138	0.4349	139	0.4138	140	0.4032
141	1.000	142	1.000	143	1.000	144	1.000	145	1.000
146	1.000	147	1.000	148	1.000	149	1.000	150	1.000
151	1.000	152	0.9981	153	0.9420	154	0.8050	155	0.6550
156	0.5435	157	0.4736	158	0.4341	159	0.4133	160	0.4030
161	1.000	162	1.000	163	1.000	164	1.000	165	1.000
166	1.000	167	1.000	168	1.000	169	1.000	170	1.000
171	1.000	172	0.9975	173	0.9389	174	0.8001	175	0.6508
176	0.5407	177	0.4720	178	0.4332	179	0.4129	180	0.4028
181	1.000	182	1.000	183	1.000	184	1.000	185	1.000
186	1.000	187	1.000	188	1.000	189	1.000	190	1.000
191	1.000	192	0.9968	193	0.9356	194	0.7950	195	0.6466
196	0.5379	197	0.4703	198	0.4323	199	0.4124	200	0.4026
201	1.000	202	1.000	203	1.000	204	1.000	205	1.000
206	1.000	207	1.000	208	1.000	209	1.000	210	1.000
211	1.000	212	0.9960	213	0.9321	214	0.7898	215	0.6423
216	0.5351	217	0.4687	218	0.4314	219	0.4120	220	0.4023
221	1.000	222	1.000	223	1.000	224	1.000	225	1.000
226	1.000	227	1.000	228	1.000	229	1.000	230	1.000
231	1.000	232	0.9950	233	0.9284	234	0.7845	235	0.6379
236	0.5322	237	0.4670	238	0.4305	239	0.4115	240	0.4021
241	1.000	242	1.000	243	1.000	244	1.000	245	1.000
246	1.000	247	1.000	248	1.000	249	1.000	250	1.000
251	1.000	252	0.9939	253	0.9244	254	0.7790	255	0.6335
256	0.5293	257	0.4653	258	0.4296	259	0.4111	260	0.4019
261	1.000	262	1.000	263	1.000	264	1.000	265	1.000
266	1.000	267	1.000	268	1.000	269	1.000	270	1.000
271	1.000	272	0.9927	273	0.9202	274	0.7733	275	0.6290
276	0.5264	277	0.4636	278	0.4287	279	0.4106	280	0.4017
281	1.000	282	1.000	283	1.000	284	1.000	285	1.000
286	1.000	287	1.000	288	1.000	289	1.000	290	1.000
291	1.000	292	0.9914	293	0.9158	294	0.7676	295	0.6245
296	0.5235	297	0.4619	298	0.4278	299	0.4102	300	0.4014
301	1.000	302	1.000	303	1.000	304	1.000	305	1.000
306	1.000	307	1.000	308	1.000	309	1.000	310	1.000
311	1.000	312	0.9899	313	0.9112	314	0.7617	315	0.6199
316	0.5205	317	0.4602	318	0.4269	319	0.4097	320	0.4012
321	1.000	322	1.000	323	1.000	324	1.000	325	1.000
326	1.000	327	1.000	328	1.000	329	1.000	330	1.000
331	1.000	332	0.9882	333	0.9063	334	0.7556	335	0.6152
336	0.5176	337	0.4585	338	0.4260	339	0.4093	340	0.4010
341	1.000	342	1.000	343	1.000	344	1.000	345	1.000
346	1.000	347	1.000	348	1.000	349	1.000	350	1.000
351	1.000	352	0.9864	353	0.9011	354	0.7495	355	0.6105
356	0.5146	357	0.4568	358	0.4251	359	0.4088	360	0.4008
361	1.000	362	1.000	363	1.000	364	1.000	365	1.000
366	1.000	367	1.000	368	1.000	369	1.000	370	1.000
371	1.000	372	0.9844	373	0.8958	374	0.7432	375	0.6058
376	0.5116	377	0.4551	378	0.4242	379	0.4084	380	0.4006
381	1.000	382	1.000	383	1.000	384	1.000	385	1.000
386	1.000	387	1.000	388	1.000	389	1.000	390	1.000
391	1.000	392	0.9823	393	0.8901	394	0.7368	395	0.6010
396	0.5086	397	0.4534	398	0.4233	399	0.4079	400	0.4003
401	1.000	402	1.000	403	1.000	404	1.000	405	1.000
406	1.000	407	1.000	408	1.000	409	1.000	410	1.000
411	1.000	412	0.9800	413	0.8842	414	0.7304	415	0.5962
416	0.5056	417	0.4517	418	0.4225	419	0.4075	420	0.4001
421	1.000	422	1.000	423	1.000	424	1.000	425	1.000
426	1.000	427	1.000	428	1.000	429	1.000	430	1.000
431	1.000	432	0.9775	433	0.8781	434	0.7238	435	0.5914
436	0.5026	437	0.4500	438	0.4216	439	0.4071	440	0.3999
441	1.000	442	1.000	443	1.000	444	1.000	445	1.000
446	1.000	447	1.000	448	1.000	449	1.000	450	1.000
451	1.000	452	0.9749	453	0.8717	454	0.7171	455	0.5865
456	0.4996	457	0.4484	458	0.4207	459	0.4066	460	0.3997

461	1.000	462	1.000	463	1.000	464	1.000	465	1.000
466	1.000	467	1.000	468	1.000	469	1.000	470	1.000
471	1.000	472	0.9721	473	0.8651	474	0.7103	475	0.5816
476	0.4966	477	0.4467	478	0.4198	479	0.4062	480	0.3995
481	1.000	482	1.000	483	1.000	484	1.000	485	1.000
486	1.000	487	1.000	488	1.000	489	1.000	490	1.000
491	1.000	492	0.9690	493	0.8582	494	0.7034	495	0.5768
496	0.4936	497	0.4450	498	0.4190	499	0.4058	500	0.3993
501	1.000	502	1.000	503	1.000	504	1.000	505	1.000
506	1.000	507	1.000	508	1.000	509	1.000	510	1.000
511	1.000	512	0.9659	513	0.8511	514	0.6965	515	0.5719
516	0.4906	517	0.4434	518	0.4181	519	0.4053	520	0.3991
521	1.000	522	1.000	523	1.000	524	1.000	525	1.000
526	1.000	527	1.000	528	1.000	529	1.000	530	1.000
531	1.000	532	0.9625	533	0.8437	534	0.6896	535	0.5670
536	0.4877	537	0.4418	538	0.4173	539	0.4049	540	0.3989
541	1.000	542	1.000	543	1.000	544	1.000	545	1.000
546	1.000	547	1.000	548	1.000	549	1.000	550	1.000
551	1.000	552	0.9590	553	0.8362	554	0.6826	555	0.5623
556	0.4849	557	0.4402	558	0.4165	559	0.4046	560	0.3987
561	1.000	562	1.000	563	1.000	564	1.000	565	1.000
566	1.000	567	1.000	568	1.000	569	1.000	570	1.000
571	0.9998	572	0.9553	573	0.8289	574	0.6762	575	0.5581
576	0.4824	577	0.4389	578	0.4159	579	0.4042	580	0.3986
581	1.000	582	1.000	583	1.000	584	1.000	585	1.000
586	1.000	587	1.000	588	1.000	589	1.000	590	1.000
591	0.9995	592	0.9521	593	0.8233	594	0.6717	595	0.5553
596	0.4809	597	0.4381	598	0.4155	599	0.4040	600	0.3985

*** NODAL DISPERSIVE FLUX VALUES ***

NODE	DISP. FLUX	NODE	DISP. FLUX	NODE	DISP. FLUX	NODE	DISP. FLUX	NODE	DISP. FLUX
1	-7.1544E-22	2	2.2457E-21	3	-1.9588E-20	4	3.3888E-20	5	-6.4186E-19
6	-7.0344E-20	7	-2.6552E-17	8	-1.1607E-16	9	-1.1233E-15	10	-4.8546E-14
11	2.0414E-13	12	-8.6371E-12	13	-9.2383E-11	14	1.0719E-10	15	1.1039E-11
16	-4.1475E-11	17	-1.2726E-13	18	1.3313E-11	19	1.8754E-11	20	2.3239E-11
21	-2.2692E-11	42	3.9980E-11	63	-1.2434E-10	84	-2.1356E-09	105	3.0719E-09
126	4.2688E-10	147	-6.2507E-11	168	1.0524E-10	189	2.1174E-09	210	-3.0089E-09
231	-4.9114E-10	252	-1.1740E-11	273	-5.1436E-12	294	-3.3107E-12	315	-5.0657E-12
336	-5.0390E-12	357	-4.7132E-12	378	-4.2007E-12	399	-3.7005E-12	420	-3.2496E-12
441	-2.8601E-12	462	-2.5273E-12	483	-2.2391E-12	504	-1.9964E-12	525	-1.7872E-12
546	-1.4255E-12	567	-1.3686E-12	588	-2.4687E-12	609	-2.8077E-12	630	6.0893E-13
651	2.4320E-12								

SUM OF ABOVE FLUX VALUES = -1.15407E-10

*** INCREMENTAL MASS BALANCE RESULTS OVER A TIME STEP ***

TOTAL DISPERSIVE FLUX RATE	-1.15407E-10
TOTAL ADVECTIVE FLUX RATE	7.98249E-07
TOTAL DISPERSIVE + ADVECTIVE FLUX RATE	7.98134E-07
RATE OF MASS DECAY	0.00000E+00
NET RATE OF MATERIAL ACCUMULATION	0.00000E+00
MASS BALANCE ERROR	7.98134E-07
NORMALIZED MASS BALANCE ERROR	9.84831E-01
RATE OF MASS ACCUMULATION DUE TO PRESSURE CHANGE	0.00000E+00

*** CUMULATIVE MASS BALANCE RESULTS ***

CUMULATIVE MATERIAL STORAGE 0.00000E+00
 CUMULATIVE MASS DECAY 0.00000E+00

*** NODAL CONCENTRATION VALUES ***

NODE	CONC. VALUE	NODE	CONC. VALUE	NODE	CONC. VALUE	NODE	CONC. VALUE	NODE	CONC. VALUE
1	0.00000E+00	2	0.00000E+00	3	0.00000E+00	4	0.00000E+00	5	0.00000E+00
6	0.00000E+00	7	0.00000E+00	8	0.00000E+00	9	0.00000E+00	10	0.00000E+00
11	0.00000E+00	12	0.00000E+00	13	0.00000E+00	14	0.00000E+00	15	0.00000E+00
16	0.00000E+00	17	0.00000E+00	18	0.00000E+00	19	0.00000E+00	20	0.00000E+00
21	0.00000E+00	22	-1.31812E-14	23	4.46815E-14	24	-1.36523E-13	25	1.22604E-12
26	-2.46997E-12	27	4.22536E-11	28	-4.85403E-12	29	1.87225E-09	30	8.63476E-09
31	8.41640E-08	32	4.07531E-06	33	-1.98056E-05	34	8.09996E-04	35	2.05549E-03
36	1.80817E-03	37	1.30035E-03	38	1.19912E-03	39	1.09035E-03	40	8.32277E-04
41	3.85049E-04	42	-2.52240E-04	43	4.73443E-14	44	-6.93833E-14	45	7.78349E-13
46	-1.03953E-12	47	2.95206E-11	48	1.76147E-11	49	1.45510E-09	50	4.43486E-09
51	1.10322E-07	52	7.68116E-07	53	2.27715E-05	54	5.77155E-04	55	-1.22195E-04
56	-9.83941E-03	57	-1.76038E-02	58	-1.59163E-02	59	-1.28320E-02	60	-9.67017E-03
61	-6.35903E-03	62	-2.87828E-03	63	7.84484E-04	64	-1.04713E-14	65	3.09903E-13
66	-9.73118E-14	67	1.49189E-11	68	2.19805E-11	69	8.59230E-10	70	2.98835E-09
71	7.24096E-08	72	3.96487E-07	73	1.92457E-05	74	2.29747E-04	75	-1.64389E-03
76	-2.01702E-02	77	-6.89580E-03	78	6.12758E-02	79	8.26649E-02	80	7.74350E-02
81	6.41221E-02	82	4.78024E-02	83	3.05884E-02	84	1.34741E-02	85	4.29648E-14
86	4.73573E-13	87	4.52065E-12	88	1.95607E-11	89	3.64947E-10	90	1.79425E-09
91	3.55759E-08	92	2.34525E-07	93	7.94900E-06	94	7.57397E-05	95	-1.05966E-03
96	-9.85225E-03	97	2.96776E-02	98	0.36743	99	0.68748	100	0.81320
101	0.87525	102	0.91684	103	0.94975	104	0.97698	105	1.0000
106	1.21996E-12	107	-1.58176E-13	108	1.62979E-11	109	7.68856E-11	110	9.38342E-10
111	1.06271E-08	112	1.03062E-07	113	2.00713E-06	114	2.16945E-05	115	-4.66540E-04
116	-4.38502E-03	117	1.36389E-02	118	0.26365	119	0.80641	120	0.98661
121	1.0050	122	1.0069	123	1.0067	124	1.0054	125	1.0031
126	1.0000	127	-7.10764E-13	128	1.19405E-11	129	-7.17416E-12	130	4.41622E-10
131	9.35417E-10	132	3.45302E-08	133	2.06084E-07	134	4.78606E-06	135	-1.60708E-04
136	-1.76779E-03	137	4.64590E-03	138	0.11909	139	0.55394	140	0.97229
141	1.0016	142	0.99852	143	0.99768	144	0.99750	145	0.99784
146	0.99868	147	1.0000	148	1.41581E-11	149	4.73750E-12	150	1.98307E-10
151	-3.13723E-10	152	8.45612E-09	153	-5.69015E-08	154	4.28961E-07	155	-4.39233E-05
156	-6.17482E-04	157	1.19864E-03	158	4.90236E-02	159	0.28358	160	0.75271
161	1.0074	162	1.0173	163	1.0165	164	1.0139	165	1.0108
166	1.0075	167	1.0039	168	1.0000	169	4.18033E-11	170	1.22564E-10
171	3.18216E-10	172	2.42169E-09	173	-1.76277E-08	174	-1.66013E-07	175	-8.98385E-06
176	-1.74866E-04	177	2.40991E-04	178	1.83710E-02	179	0.13228	180	0.45025
181	0.87626	182	1.0069	183	0.94703	184	0.92907	185	0.93532
186	0.94914	187	0.96570	188	0.98294	189	1.0000	190	1.98375E-10
191	5.97813E-10	192	2.41964E-09	193	1.24642E-08	194	-2.21334E-08	195	-8.25767E-07
196	-3.41171E-05	197	6.65940E-05	198	6.31264E-03	199	5.61564E-02	200	0.23852
201	0.59157	202	0.88147	203	0.63870	204	0.33274	205	0.20874
206	0.14543	207	0.10254	208	6.89859E-02	209	4.17237E-02	210	1.89839E-02
211	9.47789E-10	212	2.55855E-09	213	1.60130E-08	214	7.34526E-08	215	5.17626E-07
216	-4.70166E-07	217	4.63984E-05	218	2.04909E-03	219	2.17212E-02	220	0.11331
221	0.34951	222	0.67123	223	0.68116	224	0.20197	225	2.55426E-02
226	3.94283E-03	227	-9.55473E-05	228	-1.18727E-03	229	-8.45264E-04	230	6.60497E-04
231	3.09871E-03	232	3.61937E-09	233	1.16744E-08	234	7.26295E-08	235	5.01121E-07
236	3.64536E-06	237	3.38839E-05	238	6.64414E-04	239	7.73498E-03	240	4.85231E-02
241	0.18345	242	0.44216	243	0.64694	244	0.41088	245	2.97427E-02
246	-7.38940E-04	247	1.39744E-03	248	1.75576E-03	249	1.66021E-03	250	1.33531E-03

251	8.01602E-04	252	7.40686E-05	253	1.31287E-08	254	4.55654E-08	255	3.06791E-07
256	2.39572E-06	257	1.94480E-05	258	2.27641E-04	259	2.59269E-03	260	1.88781E-02
261	8.61104E-02	262	0.25571	263	0.49089	264	0.54434	265	0.22405
266	2.96757E-03	267	4.85315E-04	268	-1.53030E-05	269	-2.03726E-04	270	-2.52133E-04
271	-2.25071E-04	272	-1.29189E-04	273	3.24517E-05	274	4.45316E-08	275	1.58460E-07
276	1.16233E-06	277	9.20816E-06	278	8.30651E-05	279	8.44771E-04	280	6.76085E-03
281	3.63982E-02	282	0.13103	283	0.31614	284	0.48999	285	0.42481
286	0.12603	287	1.12081E-03	288	4.08786E-04	289	3.28429E-04	290	2.63258E-04
291	1.97615E-04	292	1.38508E-04	293	8.16889E-05	294	2.08877E-05	295	1.38177E-07
296	5.09658E-07	297	3.83948E-06	298	3.09811E-05	299	2.75806E-04	300	2.27392E-03
301	1.39899E-02	302	5.99693E-02	303	0.17731	304	0.35499	305	0.45472
306	0.32263	307	7.60970E-02	308	1.29211E-03	309	6.41623E-04	310	3.99319E-04
311	2.47214E-04	312	1.47049E-04	313	8.24812E-05	314	4.63864E-05	315	3.19605E-05
316	3.98464E-07	317	1.50419E-06	318	1.13354E-05	319	9.13109E-05	320	7.35977E-04
321	4.95898E-03	322	2.47339E-02	323	8.78504E-02	324	0.21863	325	0.37084
326	0.40369	327	0.24443	328	4.91797E-02	329	1.40693E-03	330	6.44791E-04
331	4.05854E-04	332	2.65053E-04	333	1.68134E-04	334	1.01929E-04	335	5.90236E-05
336	3.17917E-05	337	1.07569E-06	338	4.07077E-06	339	3.03850E-05	340	2.34161E-04
341	1.65129E-03	342	9.29872E-03	343	3.88779E-02	344	0.11734	345	0.25075
346	0.36799	347	0.34954	348	0.18677	349	3.35848E-02	350	1.32653E-03
351	6.01473E-04	352	3.76861E-04	353	2.42640E-04	354	1.51402E-04	355	9.01354E-05
356	5.18911E-05	357	2.97364E-05	358	2.71738E-06	359	1.01792E-05	360	7.40176E-05
361	5.26971E-04	362	3.23361E-03	363	1.55385E-02	364	5.57177E-02	365	0.14566
366	0.27212	367	0.35239	368	0.29875	369	0.14454	370	2.39016E-02
371	1.17931E-03	372	5.37437E-04	373	3.36955E-04	374	2.17501E-04	375	1.36080E-04
376	8.13406E-05	377	4.69398E-05	378	2.65030E-05	379	6.43370E-06	380	2.36348E-05
381	1.63873E-04	382	1.05803E-03	383	5.68046E-03	384	2.36945E-02	385	7.41519E-02
386	0.17066	387	0.28328	388	0.32935	389	0.25387	390	0.11336
391	1.75409E-02	392	1.02485E-03	393	4.74537E-04	394	2.98224E-04	395	1.92210E-04
396	1.19907E-04	397	7.14542E-05	398	4.11676E-05	399	2.33468E-05	400	1.43223E-05
401	5.10343E-05	402	3.31352E-04	403	1.92752E-03	404	9.13371E-03	405	3.35443E-02
406	9.29605E-02	407	0.19104	408	0.28584	409	0.30279	410	0.21540
411	9.00552E-02	412	1.31755E-02	413	8.85851E-04	414	4.18217E-04	415	2.63497E-04
416	1.69751E-04	417	1.05731E-04	418	6.29226E-05	419	3.62206E-05	420	2.05023E-05
421	3.00498E-05	422	1.02657E-04	423	6.16897E-04	424	3.23373E-03	425	1.36496E-02
426	4.46801E-02	427	0.11104	428	0.20632	429	0.28175	430	0.27532
431	0.18294	432	7.23871E-02	433	1.00761E-02	434	7.66769E-04	435	3.69597E-04
436	2.33453E-04	437	1.50271E-04	438	9.34036E-05	439	5.54765E-05	440	3.18921E-05
441	1.80446E-05	442	5.95185E-05	443	1.93029E-04	444	1.06714E-03	445	5.05791E-03
446	1.91892E-02	447	5.65940E-02	448	0.12753	449	0.21661	450	0.27288
451	0.24854	452	0.15577	453	5.88048E-02	454	7.81622E-03	455	6.66677E-04
456	3.27865E-04	457	2.07761E-04	458	1.33642E-04	459	8.29023E-05	460	4.91464E-05
461	2.82145E-05	462	1.59450E-05	463	1.11491E-04	464	3.40930E-04	465	1.73041E-03
466	7.45256E-03	467	2.56301E-02	468	6.87640E-02	469	0.14187	470	0.22237
471	0.26080	472	0.22334	473	0.13307	474	4.82195E-02	475	6.13331E-03
476	5.82430E-04	477	2.93046E-04	478	1.85789E-04	479	1.19306E-04	480	7.38210E-05
481	4.36648E-05	482	2.50275E-05	483	1.41266E-05	484	1.98028E-04	485	5.68782E-04
486	2.65181E-03	487	1.04361E-02	488	3.27927E-02	489	8.07227E-02	490	0.15379
491	0.22426	492	0.24677	493	0.20013	494	0.11408	495	3.98619E-02
496	4.85367E-03	497	5.11428E-04	498	2.58748E-04	499	1.65040E-04	500	1.06100E-04
501	6.56166E-05	502	3.88041E-05	503	2.22615E-05	504	1.25955E-05	505	3.34613E-04
506	9.01584E-04	507	3.86947E-03	508	1.39961E-02	509	4.04748E-02	510	9.21054E-02
511	0.16322	512	0.22299	513	0.23172	514	0.17903	515	9.81338E-02
516	3.31604E-02	517	3.87212E-03	518	4.46269E-04	519	2.42549E-04	520	1.54862E-04
521	9.90783E-05	522	6.08621E-05	523	3.57002E-05	524	2.02609E-05	525	1.12759E-05
526	5.39959E-04	527	1.36581E-03	528	5.41365E-03	529	1.81006E-02	530	4.84906E-02
531	0.10268	532	0.17030	533	0.21923	534	0.21627	535	0.15993
536	8.46214E-02	537	2.77418E-02	538	3.07482E-03	539	4.22243E-04	540	1.98899E-04
541	1.22841E-04	542	7.77395E-05	543	4.75535E-05	544	2.79118E-05	545	1.59393E-05
546	8.99371E-06	547	8.35393E-04	548	1.98875E-03	549	7.30921E-03	550	2.27168E-02
551	5.67082E-02	552	0.11236	553	0.17529	554	0.21356	555	0.20074
556	0.14261	557	7.30617E-02	558	2.30775E-02	559	2.52917E-03	560	2.11994E-04
561	1.24230E-04	562	8.51819E-05	563	5.69935E-05	564	3.64785E-05	565	2.25426E-05
566	1.38068E-05	567	8.63446E-06	568	1.24334E-03	569	2.79588E-03	570	9.57432E-03
571	2.78141E-02	572	6.50608E-02	573	0.12120	574	0.17851	575	0.20636
576	0.18521	577	0.12627	578	6.25001E-02	579	1.95727E-02	580	1.45096E-03
581	4.33384E-04	582	3.12896E-04	583	2.13448E-04	584	1.38507E-04	585	8.50395E-05
586	4.97017E-05	587	2.80988E-05	588	1.55757E-05	589	1.77900E-03	590	3.79624E-03
591	1.21682E-02	592	3.32442E-02	593	7.33113E-02	594	0.12911	595	0.18018

596	0.19759	597	0.16865	598	0.11069	599	5.31109E-02	600	1.31291E-02
601	2.33527E-03	602	8.50731E-04	603	4.98180E-04	604	3.15871E-04	605	1.97730E-04
606	1.17807E-04	607	6.63606E-05	608	3.54253E-05	609	1.77141E-05	610	2.40686E-03
611	4.90100E-03	612	1.48194E-02	613	3.83016E-02	614	8.02882E-02	615	0.13485
616	0.17958	617	0.18701	618	0.14884	619	8.63869E-02	620	3.41055E-02
621	1.41841E-02	622	2.27915E-03	623	3.73662E-04	624	9.34260E-05	625	2.94709E-05
626	8.66427E-06	627	5.32039E-07	628	-2.57568E-06	629	-3.59388E-06	630	-3.84180E-06
631	2.72945E-03	632	5.45476E-03	633	1.60570E-02	634	4.06600E-02	635	8.32636E-02
636	0.13682	637	0.17855	638	0.18128	639	0.13795	640	7.36074E-02
641	8.94022E-03	642	-2.42159E-03	643	-2.67358E-03	644	-1.67204E-03	645	-1.06706E-03
646	-6.75646E-04	647	-4.15006E-04	648	-2.41236E-04	649	-1.31744E-04	650	-6.71419E-05
651	-3.06796E-05								

***** SAMFT2D HAS SOLVED THE PROBLEM *****

 *** CPU TIME USED: 24.67 SECS. ***

- 5) Steady-state simulation result:
 - mass balance information
 - nodal concentration values.
- 6) CPU time for the simulation (for 80386 computer).

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