VAM2D – Variably Saturated Analysis Model in Two Dimensions

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Version 5.2 With Hysteresis and Chained Decay Transport

Documentation and User's Guide

Prepared by
P. S. Huyakorn, J. B. Kool, Y. S. Wu

HydroGeoLogic, Inc.

Prepared for
U.S. Nuclear Regulatory Commission

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ABSTRACT

This report documents a two-dimensional finite element model, VAM2D, developed to simulate water flow and solute transport in variably saturated porous media. Both flow and transport simulation can be handled concurrently or sequentially. The formulation of the governing equations and the numerical procedures used in the code are presented. The flow equation is approximated using the Galerkin finite element method. Nonlinear soil moisture characteristics and atmospheric boundary conditions (e.g., infiltration, evaporation and seepage face), are treated using Picard and Newton-Raphson iterations. Hysteresis effects and anisotropy in the unsaturated hydraulic conductivity can be taken into account if needed. The contaminant transport simulation can account for advection, hydrodynamic dispersion, linear equilibrium sorption, and first-order degradation. Transport of a single component or a multi-component decay chain can be handled. The transport equation is approximated using an upstream weighted residual method. Several test problems are presented to verify the code and demonstrate its utility. These problems range from simple one-dimensional to complex two-dimensional and axisymmetric problems.

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 restarting procedures.

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EXECUTIVE SUMMARY

Proper disposal of low-level radioactive waste (LLW) in the United States has been a problem with increasingly difficult technical and social challenges for several years. Under the 1980 Low-Level Waste Policy Act and Amendments, individual states, as well as groups of states, have been seeking to establish new disposal sites. Any new site to be established must meet applicable federal and state regulatory criteria to become licensed, such as 10 CFR Part 61 under the authority of Nuclear Regulatory Commission.

10 CFR Part 61.5 contains criteria covering many technical requirements for low-level waste siting. The first and most prominent hydrogeologic criterion states "the disposal site shall be capable of being characterized, modeled, analyzed, and monitored." The regulations also indicate that disposal zones should be well above the water-table fluctuation zone, unless very restrictive conditions are met which would allow disposal below the water table. One of the principal reasons that modeling is required, is to demonstrate that radionuclide migration away from the disposed waste, either in liquid or gaseous state, will meet regulatory concentration limits at the boundary of the site or points of exposure.

Current regulations require site performance criteria to be satisfied for a period of at least 500 years. Most operating and planned LLW disposal facilities are situated in the unsaturated zone above the water table. Problems with existing LLW disposal facilities have often been associated with unfavorable hydrologic conditions at the site (Robertson, 1984). Consequently, a subsurface flow and radionuclide transport model, capable of simulating a wide range of conditions, is an essential tool for performance assessment of a planned LLW facility.

Several states (such as Pennsylvania, New York, Illinois, California, Texas, and North Carolina) recently initiated programs to select, characterize, license, and operate new disposal sites. Other state and federal agencies will probably begin seeking additional sites within the next few years. Although a variety of disposal methods are being considered, most are focused on disposal above the water table. Regardless of the location or disposal method chosen, most new sites will require modeling of water flow and solute transport through the unsaturated zone to the water table. However, our ability to model these processes in most environments is limited by capabilities of existing models. Existing models such as UNSAT2, TRACR3D, TRUST, SUTRA, TOUGH, FEMWATER/FEMWASTE, GS2/GS3, and SATURN all have rather narrow limits in numerical stability, robustness, user-friendliness, or in other characteristics which inhibit their applicability to many real-world conditions existent at potential LLW sites currently under consideration. Some of the conditions which have previously been unfeasible or extremely difficult to model include:

- fully three-dimensional heterogeneous flow and transport with highly variable hydraulic properties;

- strong hysteretic and/or anisotropic conditions;
- nonlinear sorption and multi-species chain decay;
- highly variable transient moisture conditions, ranging from extremely dry to very wet and/or highly heterogeneous hydraulic properties;
- dual porosity fractured/porous media; and
- unusual boundary conditions and disposal concepts such as engineered two- and three-dimensional wicking schemes, capillary barrier trench cap designs, deep-boring emplacement, and intermediate depth burial.

Conditions likely to be encountered at LLW disposal sites include dry conditions with very low rates of liquid movement. Especially for the shallow land burial scenario, evapotranspiration losses may have a large effect on the site hydrology. Under arid conditions, this process may represent a very large portion of the total water balance and must be adequately accounted for in a model. In addition to passive movement with the water phase, the migration of radionuclides will be affected by sorption reactions with the solid phase matrix and chained decay reactions. These processes should also be accounted for in a model.

There is a clear regulatory need for a more suitable low-level waste site hydrogeologic model, as well as a broader technical need in nuclear and hazardous waste management and in general hydrology. The VAM2D model described in this report is intended to be useful in the selection, characterization, and design stages of a waste disposal facility, for instance by allowing evaluation of the effectiveness of different cap designs. The model will further enable more accurate prediction of repository performance and compliance assessment. The model advances the state-of-the-art in unsaturated zone modeling by incorporating features that are not available in current models.

Like all other modeling codes, the VAM2D model described herein has its limitations, such as two dimensionality. This code represents only one stage of an evolving modeling program which is eventually intended to accommodate three-dimensional flow, vapor phase, and energy transport, fractures and macro pores, and other enhancements.

The special capabilities and advantages of the version presented in this document include the following:

- accounts for moisture uptake and retraction by plants in the root zone;
- simulates flow and transport in saturated as well as unsaturated zones;
- can solve flow and transport equations simultaneously or sequentially;

- accommodates a wide range of field conditions including highly nonlinear moisture characteristics, anisotropy, heterogeneity, and highly transient boundary conditions;
- accounts for multiple-component and multiple-chain decay reactions and species;
- computes hysteretic effects on flow due to wetting and drying cycles;
- computes effects of variable anisotropic hydraulic conductivities on flow in stratified media;
- includes other, more standard features such as linear equilibrium sorption and dispersion; and
- interfaces with a PC-based, user-friendly pre-processor which greatly facilitates problem set-up, reduces data modification time and eliminates inadvertent input format errors.

The principal objective in developing this version of VAM2D was to create a very versatile code which can be reliably applied to a wide range of low-level radioactive waste site conditions (and related types of sites) that have hitherto been either unamenable to modeling or extremely difficult to model. A second objective was to develop a code that is relatively easy to use on microcomputers by a large number of potential users with appropriate technical background. Finally, it is intended that this code have wide spread usefulness in application to situations other than LLW sites (e.g., hazardous waste, mixed-waste, and municipal landfill and electric power generation waste sites).

PART I

THEORY, MATHEMATICAL MODEL, AND CODE DESIGN

1 INTRODUCTION

1.1 BACKGROUND AND PURPOSE OF THE CODE

VAM2D is a two-dimensional, finite element code developed to simulate moisture movement and solute transport in variably saturated porous media. The code is capable of simulating a wide range of conditions commonly encountered in the field. Simulations can be performed in a vertical cross-section, or an axisymmetric configuration. Both flow and transport simulations can be handled 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 simple rectangular or orthogonal curvilinear elements to analyze problems involving highly nonlinear soil moisture characteristics. Many types of boundary conditions can be accommodated: 1) water table conditions, 2) evaporation and nonponding infiltration, 3) water uptake by plant roots, 4) vertical recharge of the water table, 5) pumping and injection wells, and 6) seepage faces.

The model formulation used in VAM2D is a descendant of the formulation used in the SATURN code presented by Huyakorn, et al. (1984, 1985). HydroGeoLogic, Inc. has recently enhanced certain portions of the published algorithms and their coding to achieve greater flexibility, wider capability, and more robust numerical performances when dealing with some difficult cases. Where possible, the new VAM2D code has been rigorously checked against available analytical or semi-analytical solutions and similar numerical codes including UNSAT2, FEMWATER/FEMWASTE, SATURN, and VADOFT. A variety of field simulation problems described in the works of Huyakorn et al. (1984, 1985, 1987), Enfield et al. (1983), and Carsel et al. (1985) have been used to validate VAM2D and demonstrate its utility. Additional simulation problems are described in this report.

1.2 OVERVIEW OF CODE CAPABILITIES AND SALIENT FEATURES

Multidimensional modeling of water flow and waste migration in variably saturated subsurface systems can be a formidable task unless one is equipped with a proper code that accommodates various field conditions. Recognizing this point, VAM2D 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. VAM2D can perform transient analyses or single step steady-state analyses of both variably saturated water flow and solute transport problems. If the flow and transport problems are associated, a dual simulation can be made by solving the problems concurrently or sequentially in a single computer run.

2. The finite element formulation and nonlinear solution procedures in VAM2D are based on the 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. VAM2D uses highly efficient matrix computational and solution techniques. This feature makes the code attractive to use on a minicomputer or even a personal computer.

4. The flow simulator of VAM2D can handle various boundary conditions and physical processes including infiltration, evaporation, plant root uptake, seepage faces, well pumping and recharging, and varying water table conditions. Temporal variations of transient head and flux boundary conditions can be handled conveniently using either continuous piecewise linear representations or discontinuous (stepped) representations. Additionally, hysteretic moisture characteristics as well as variable anisotropy in the hydraulic conductivity of the unsaturated soil can be accounted for if needed. Presently, the effects of these phenomena on moisture movement and solute transport in the field are not clearly understood. In view of this, the VAM2D code may be used as a modeling tool to supplement field investigation or other research study of complex flow and transport behavior in variably saturated media.

5. The transport simulator of VAM2D can handle both single-species and chained decay transport problems. Its formulation is designed to have upstream weighting capability to circumvent numerical oscillations. The scheme can accommodate straight and branched chains as well as decaying contaminant sources. Both pulse and step releases of contaminants from each source can be simulated. These capabilities make it advantageous to use VAM2D in the prediction of fate and transport of reactive chemicals and radioactive elements.

1.3 DESCRIPTION OF CODE CHANGES AND ENHANCEMENTS IN VAM2D VERSION 5.2

This document is a revision of the documentation and user's manual to VAM2D, version 5.0 which was published as NUREG/CR-5352 (1989). A number of enhancements have been incorporated in the code as part of work conducted for the USNRC as part of a project entitled "Validation and testing of the VAM2D computer code". The most important changes are listed below:

- Revised computational schemes for improved water and solute mass balance under very nonlinear conditions
- Allow curvilinear as well as rectangular grid

- Boundary conditions now allow seepage faces and free drainage outflow boundaries
- Infiltration boundaries along the soil surface now allow for time-varying precipitation
- VAM2D now incorporates an adaptive time stepping scheme for variably saturated flow simulations in which the time step is automatically adjusted to achieve optimal computational efficiency
- Simulation output can now be obtained at user-specified time values, rather than just at fixed time step intervals
- Velocities are written out in a format that allows SURFER™ to create plots of velocity vectors
- The capacity of VAM2D has been increased to handle problems with up to 5000 nodes.

1.4 APPLICABILITY OF THE CODE

The VAM2D code has many practical applications. Typical examples include the following:

- Performance assessment of subsurface waste disposal facilities for radioactive and hazardous waste including flow pathway delineation and contaminant migration assessment.
- Investigation of moisture movement and evapotranspiration in the unsaturated zone including hysteresis plant water uptake in the root zone.
- Watershed studies - used to predict the response of unconfined watersheds to different schemes of drainage or to infiltration and evaporation. The code computes spatial and temporal variations in the pressure head, water saturation, and flow rate across specified flow boundaries.
- Assessment of well performance and pumping test analysis - used to analyze flow in the vicinity of pumped wells, to predict well performance, and to prepare type curves for evaluation of pumping test data.

- Mine dewatering investigations - used to predict the change in elevations of water table or phreatic surface in response to mine dewatering operations. These predictions can be obtained by performing areal or cross-sectional analyses of unconfined flow problems.
- Contaminant migration assessment - used to predict leakage rates and flow fields in unconfined aquifers underlying sewage ponds, surface impoundments, and landfills. VAM2D can simulate contaminant transport in variably or fully saturated porous media.

1.5 CODE USER REQUIREMENTS

In order to apply the VAM2D code effectively, the user will need:

- a thorough understanding of hydrogeological principles
- working knowledge of finite element 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.

Throughout this manual it is assumed that the reader has a good working knowledge of the finite element technique for solving groundwater flow and transport problems. The finite element method is a powerful, but also complex numerical technique. This documentation is not a tutorial on the finite element method or numerical modeling in general. Useful general texts on the use of numerical groundwater models include: Anderson and Wang (1982), de Marsily (1986) and Bear and Verruyt (1987). An in-depth introduction to the finite element method as applied to groundwater modeling problems has been published by the American Geophysical Union as Water Resources Monograph #13 (Istok, 1990).

1.6 COMPUTER EQUIPMENT REQUIREMENTS

VAM2D 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 Intel386 and PRIME minicomputers using the FORTRAN 77 compiler developed by the University of Salford, United Kingdom. Installation of the code has also been made on IBM,

CRAY, VAX, micro-VAX, SUN, MIPS and INTEL 80386/486 computers with standard FORTRAN 77 compilers. In order to compile and run the source code on a PC 386 machine, a computer equipped with at least 4 megabytes of core memory, a protected mode FORTRAN 77 compiler, and a 80387 or Weitek math co-processor is required.

2 GOVERNING MATHEMATICAL MODELS

2.1 PROCESS AND GEOMETRY

VAM2D performs two-dimensional or axisymmetric finite element simulations of water flow and/or solute transport in variably saturated and fully saturated porous media. The code employs state-of-the-art numerical technology to provide efficient steady-state and transient solutions of practical problems encountered in the investigation, mitigation and remediation of soil and groundwater contamination due to disposal of chemical and/or nuclear wastes. The steady-state analysis is performed by disregarding all storage terms of the governing equations thus avoiding the necessity of time marching. The transient analysis is performed by time marching until the prescribed number time steps are reached. For water flow simulations, VAM2D can handle a variety of boundary conditions including infiltration, evaporation, seepage faces, and plant root extraction. The code can also accommodate severely nonlinear soil moisture characteristics and hysteresis as well as anisotropy in variably saturated hydraulic conductivity. For solute transport simulations, VAM2D accounts for advection, hydrodynamic dispersion, equilibrium sorption, first-order decay, and zero-order production.

Transport of a single component or straight and branched decay chains of parent-daughter components can be handled.

The user is permitted to employ the following coordinates:

- two-dimensional Cartesian coordinates (x,y) with the (x-y) plane being vertical or horizontal
- axisymmetric cylindrical coordinates with (x,y) corresponding to radial and vertical coordinates (r,z)
- two-dimensional Cartesian coordinates (x,y) with the (x-y) plane being vertical but sloping.

2.2 GOVERNING AND SUPPLEMENTARY EQUATIONS FOR VARIABLY SATURATED FLOW

For variably saturated flow analysis, the VAM2D code uses pressure head as the dependent variable. The governing equation for water flow in a variably saturated soil is written as:

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

where ρ_w is the density of water, ψ is the 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.

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

$$\frac{\partial}{\partial x_i} \left[K_{ij} k_{rw} \left(\frac{\partial \psi}{\partial x_j} + e_j \right) \right] = (S_w S_s + \frac{dS_w}{d\psi}) \frac{\partial \psi}{\partial t} - q \quad (2.2)$$

or

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

where η is a coefficient defined as

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

The coefficient S_s in equation (2.4) is known as specific storage and is defined as $S_s = \rho_w g (\phi \beta + \alpha)$, where g is the gravitational constant and α and β are coefficients of compressibility of the porous medium and water, respectively. The off-diagonal components of the saturated conductivity tensor, $K_{12} = K_{21}$, will be zero if the coordinate system coincides with the principal axes of anisotropy of the hydraulic conductivity. An example is the x_1 -direction parallel to stratification and x_2 direction normal to stratification. Otherwise, these off-diagonal components will be non-zero.

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

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

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

and

$$v_i n_i = -v_n \text{ on } B_2 \quad (2.7a)$$

where ψ_o is the initial head value, B_1 is the portion of the flow boundary where ψ is prescribed as $\tilde{\psi}$, 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.

A special case of condition (2.7a) may exist along the lower boundary in a vertical cross-sectional simulation. Rather than specifying the pressure head itself or a given water flux, a zero-pressure head gradient can be specified:

$$\frac{\partial \psi}{\partial x_2} = 0 , \quad (2.7b)$$

where x_2 is the vertical coordinate. This condition approximates a freely draining soil profile.

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

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

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, 1980):

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

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

Van Genuchten (1980) has shown that equations (2.8a) and (2.8b) will yield approximately the same relative permeability curves if the parameter n is chosen such that

$$n = 1 + 2/\gamma$$

Using the relation $\gamma = 1 - 1/\beta$, the above relationship can also be written as:

$$n = 3 + 2/(\beta - 1) .$$

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

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

2.3 DESCRIPTION OF HYSTERESIS AND UNSATURATED ANISOTROPY

Although generally ignored in variably saturated simulation models, the saturation-pressure head relation of soils exhibits hysteresis. At a given pressure head, saturation will be higher when the soil is draining from saturation than it is when the soil is rewetting. As a consequence, hysteresis may have a significant effect on flow as well as contaminant transport in the unsaturated zone when the soil is alternately wetting and draining. An example of such a situation is a waste disposal bed which receives waste water at intervals in time.

Because of hysteresis, the $S_w(\psi)$ relation cannot be described by a single curve. Instead, a family of curves is required, bounded by a main drying curve and main wetting curve. The actual saturation at any point in the soil during unsaturated flow is a function, not only of pressure head, but also of the entire wetting-drying history of the soil. The approach used in VAM2D to simulate hysteresis is based on the use of Eq. (2.9) to describe the $S_w(\psi)$ relation, but modifying the equation to allow for different wetting and drying curves. This is achieved by retaining the form of (2.9) for both wetting and drying $S_w(\psi)$ curves but assigning different values of the parameters α , β and γ to wetting and drying curves. For a hysteretic simulation, the VAM2D code computes the appropriate $S_w(\psi)$ relation for all intermediate scanning curves from the specified parameters for the two boundary curves using the procedure developed by Kool and Parker (1987) which is summarized in Section 3.2.5.

Many natural soils and other geologic media exhibit some degree of stratification leading to anisotropy of hydraulic conductivity, with higher conductivity in the direction parallel to stratification than perpendicular to stratification. This anisotropy is usually expressed as a ratio

$$r = \frac{K_{11}}{K_{22}} \quad (2.11)$$

where the index 1 indicates the direction parallel to stratification and 2 corresponds to the perpendicular direction. As expressed by (2.11), the anisotropy ratio is constant and independent of saturation. Recent research (e.g., Yeh et al., 1985; Mantoglou and Gelhar, 1987; McCord et al., 1988) suggests that in reality, the relative permeability k_{rw} may be subject to strong anisotropy. This research indicates that for unsaturated conditions, the

hydraulic conductivity anisotropy is inversely related to the degree of water saturation. Assuming an exponential $k_{rw}(\psi)$ relation and using stochastic theory, Yeh et al. (1985) have developed the following expression for anisotropy as a function of pressure head for layered soils with a mean unit downward hydraulic gradient

$$r(\psi) = \frac{(Kk_{rw})_{11}}{(Kk_{rw})_{22}} = \exp \left[\frac{\sigma_f^2 + \sigma_a^2 \bar{\psi}^2}{1 + \mu \bar{a} \cos \omega} \right] \quad (2.12)$$

where σ_f^2 is the variance of the log saturated conductivity ($\ln K$), a is the slope of the $\ln(k_{rw})$ versus ψ curve, $\bar{a}$ is the mean value of a , σ_a^2 is the variance of $\bar{a}$, $\bar{\psi}$ is the mean value of ψ , μ is the spatial correlation length, and ω is the angle between the soil layer stratification and the horizontal.

Equation (2.12) indicates that anisotropy increases as an exponential function of the second power of pressure head. According to (2.12) anisotropy will also be more pronounced when the spatial variability of hydraulic conductivity increases and the correlation length, μ , decreases. The concept of variable anisotropy is based on mainly theoretical considerations and the predictive value of (2.12) has not been extensively tested. Nevertheless, McCord et al. (1988) have experimentally observed patterns of water and solute plume migration in a hill slope infiltration study that are similar to results obtained by computer simulation which incorporated (2.12) to model variable anisotropy. VAM2D has an option to use (2.12) to incorporate variable anisotropy in unsaturated flow modeling. Details of the implementation procedure are given in Section 3.2.5.

2.4 ATMOSPHERIC BOUNDARY CONDITIONS AND PLANT ROOT UPTAKE

Atmospheric boundaries may correspond to soil-air interfaces where evaporation or infiltration occurs. They may also correspond to seepage faces through which water seeps from the saturated portion of the flow domain.

Along infiltration and evaporation boundaries, conditions may change from the Dirichlet (prescribed head) to the Neuman (prescribed flux) type. In the absence of surface ponding, a numerical solution is obtained by maximizing the absolute value of the flux (while maintaining the appropriate sign) subject to the following requirements (Hanks et al., 1969; Neuman et al., 1974):

$$|v_i n_i| \leq |E_s^*| \quad (2.13)$$

and

$$\psi_L \leq \psi \leq 0 \quad (2.14)$$

where E_s^* is the maximum potential surface flux under the prevailing atmospheric conditions, and ψ_L is the minimum pressure head allowed under the prevailing soil conditions.

Along a seepage face the condition of zero atmospheric pressure head prevails. However, the length of the seepage face is not known a priori. It must be determined during a simulation so that the water efflux condition (outflow only) is satisfied on the seepage face.

For cases involving plant root uptake, the sink term in the governing equation (2.3) is represented by the following equation (Feddes et al., 1974):

$$q = K_{11} k_{rw} (\psi - \psi_r) b'$$

where ψ_r is the root pressure head, and b' is a root effectiveness function.

2.5 GOVERNING EQUATIONS AND INITIAL AND BOUNDARY CONDITIONS FOR THE SOLUTE TRANSPORT MODEL

2.5.1 Single-Species Transport

The governing equation for two-dimensional transport of a non-conservative single component in a variably saturated soil takes the form

$$\begin{aligned} \frac{\partial}{\partial x_i} (D_{ij} \frac{\partial c}{\partial x_j}) - \frac{\partial}{\partial x_i} (v_i c) = \frac{\partial}{\partial t} [\phi S_w c + \rho_s (1-\phi) c_s] - q c^* \\ + \lambda [\phi S_w c + \rho_s (1-\phi) c_s] \end{aligned} \quad (2.15)$$

where D_{ij} is the apparent hydrodynamic dispersion tensor, c is solute concentration in the fluid, v_i is the Darcy velocity, 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 solution concentration is described by a linear equilibrium isotherm, Equation 2.15 can be expressed as

$$\begin{aligned} \frac{\partial}{\partial x_i} (D_{ij} \frac{\partial c}{\partial x_j}) - \frac{\partial}{\partial x_i} (v_i c) = \frac{\partial}{\partial t} \left[\phi S_w \left(1 + \frac{\rho_s(1-\phi)k_d}{\phi S_w} \right) c \right] - qc^* \\ + \lambda \phi S_w \left[1 + \frac{\rho_s(1-\phi)k_d}{\phi S_w} \right] c \end{aligned} \quad (2.16)$$

where k_d is the equilibrium constant.

Equation 2.16 reduces to

$$\begin{aligned} \frac{\partial}{\partial x_i} (D_{ij} \frac{\partial c}{\partial x_j}) - \frac{\partial}{\partial x_i} (v_i c) = \frac{\partial}{\partial t} (\phi S_w R c) \\ + \lambda \phi S_w R c - q c^* \end{aligned} \quad (2.17)$$

where R is the retardation factor defined as

$$R = 1 + \frac{\rho_s(1-\phi)k_d}{\phi S_w} = 1 + \frac{\rho_B k_d}{\phi S_w} \quad (2.18)$$

with the bulk density ρ_B being defined as $(1-\phi)\rho_s$. Expanding the convective and mass accumulation terms of Equation 2.17 and using the continuity equation of fluid flow, one obtains

$$\begin{aligned} \frac{\partial}{\partial x_i} (D_{ij} \frac{\partial c}{\partial x_j}) - v_i \frac{\partial c}{\partial x_i} = \phi S_w R \frac{\partial c}{\partial t} + c \frac{\partial}{\partial t} (\phi S_w) + c \frac{\partial}{\partial t} (\rho_B k_d) \\ - c \frac{\partial}{\partial t} (\phi S_w) + q(c - c^*) + \lambda \phi S_w R c \end{aligned} \quad (2.19)$$

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

$$\frac{\partial}{\partial x_i} (D_{ij} \frac{\partial c}{\partial x_j}) - v_i \frac{\partial c}{\partial x_i} = \phi S_w R \left(\frac{\partial c}{\partial t} + \lambda c \right) + q(c - c^*) \quad (2.20)$$

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):

$$D_{11} = \frac{\alpha_L (v_1)^2}{|v|} + \frac{\alpha_T (v_2)^2}{|v|} + D^o \quad (2.21a)$$

$$D_{22} = \frac{\alpha_L (v_2)^2}{|v|} + \frac{\alpha_T (v_1)^2}{|v|} + D^o \quad (2.21b)$$

$$D_{12} = D_{21} = (\alpha_L - \alpha_T) \frac{v_1 v_2}{|v|} \quad (2.21c)$$

where α_L and α_T are longitudinal and transverse dispersivities, respectively, and D^o is the apparent molecular diffusion coefficient. D^o is defined as $\phi \tau D_m$, where D_m is the free-water molecular diffusion coefficient and τ is a saturation dependent tortuosity factor. VAM2D uses the Millington-Quirk (1961) relation to evaluate τ :

$$\tau = \phi^{4/3} S_w^{10/3} \quad (2.21d)$$

Equation 2.20 is the final 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 2.20 are as follows:

$$c(x_1, x_2, 0) = c_o \quad (2.22a)$$

$$c(x_1, x_2, t) = \tilde{c} \quad \text{on } B_1 \quad (2.22b)$$

$$D_{ij} \frac{\partial c}{\partial x_j} n_i = q_c^D \quad \text{on } B_2 \quad (2.22c)$$

$$D_{ij} \frac{\partial c}{\partial x_j} n_i - v_i n_i c = q_c^T \quad \text{on } B_3 \quad (2.22d)$$

where B_1 is the portion of the boundary where concentration is prescribed as $\tilde{c}$, 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.

2.5.2 Chained-Decay Transport

Transport of a chain of decaying solute species is described by the following set of equations:

$$\begin{aligned} \frac{\partial}{\partial x_i} \left(D_{ij} \frac{\partial c_\ell}{\partial x_j} \right) - v_i \frac{\partial c_\ell}{\partial x_i} &= \phi S_w R_\ell \left(\frac{\partial c_\ell}{\partial t} + \lambda_\ell c_\ell \right) + q(c_\ell - c_\ell^*) \\ &- \sum_{m=1}^M \phi S_w \xi_{\ell m} R_m \lambda_m c_m, \end{aligned} \quad (2.23)$$

$$\ell = 1, \dots, n_c$$

where subscript ℓ denotes the chemical component, n_c is the number of components in the chain, $\xi_{\ell m}$ is the mass fraction of (parent) component m transforming to (daughter) component ℓ , and M is the number of parents transforming to ℓ .

For radioactive decay, λ_ℓ is related to the half-life by the following equation:

$$\lambda_\ell = \frac{\ln 2}{t_{1/2, \ell}} \quad (2.24)$$

Initial and boundary conditions associated with (2.23) may be expressed as

$$c_\ell(x_1, x_2, 0) = c_{\ell o} \quad (2.25)$$

$$c_\ell(x_1, x_2, t) = \tilde{c}_\ell \quad \text{on } B_1 \quad (2.26a)$$

$$D_{ij} \frac{\partial c_\ell}{\partial x_j} n_i = q_{c\ell}^D \quad \text{on } B_2 \quad (2.26b)$$

$$D_{ij} \frac{\partial c_\ell}{\partial x_j} n_i - v_i n_i c_\ell = q_{c\ell}^T \quad \text{on } B_3 \quad (2.26c)$$

For a decaying source, the prescribed concentration $\tilde{c}_\ell$ (or prescribed contaminant flux $q_{c\ell}^T$) is time-dependent and governed by Bateman's equation:

$$\frac{d\tilde{c}_\ell}{dt} = -\lambda_\ell \tilde{c}_\ell + \sum_{m=1}^M \xi_{\ell m} \lambda_m \tilde{c}_m \quad (2.27)$$

subject to

$$\tilde{c}_\ell(t=0) = \tilde{c}_\ell^o \quad (2.28)$$

For a n_c -member chain, the general solution of (2.27) subject to (2.28) may be written in the form:

$$\tilde{c}_\ell = \tilde{c}_\ell^o e^{-\lambda_\ell t} + \xi_{\ell, \ell-1} \lambda_{\ell-1} \tilde{c}_{\ell-1}^o \sum_{m=\ell-1}^{\ell} \frac{e^{-\lambda_m t}}{\prod_{\substack{k=\ell-1 \\ k \neq m}} (\lambda_k - \lambda_m)}$$

$$\begin{aligned}
& + \dots + \xi_{\ell, \ell-1} \lambda_{\ell-1} \xi_{\ell-1, \ell-2} \dots \xi_{21} \lambda_1 \tilde{c}_1^0 \\
& \cdot \sum_{m=1}^{\ell} \frac{e^{-\lambda_m t}}{\prod_{\substack{k=1 \\ k \neq m}}^{\ell} (\lambda_k - \lambda_m)}
\end{aligned} \tag{2.29}$$

where ℓ ranges from 1 to n_c , and $\tilde{c}_\ell^0$ ($\ell=1, \dots, n_c$) are initial source concentrations of components 1 through n_c . Note that λ_ℓ ($\ell = 1, \dots, n_c$) are source decay coefficients. In the VAM2D code these source decay coefficients may be assumed to be the same as or different from the decay coefficients in the governing advective-dispersive transport equations (2.23).

Equation (2.29) assumes a step release of dissolved contaminants at the source (i.e., all of the waste material begins to dissolve at time $t=0$ and distribution is allowed to proceed continuously at a uniform rate). For the case of pulse or band release of leach duration T , the right hand side of (2.29) must be modified by multiplying by the following factor:

$$f = [U(t) - U(t-T)] \tag{2.30}$$

where $U(t-T)$ is the Heaviside unit function defined as

$$U(t-T) = \begin{cases} 1, & t \geq T \\ 0, & t < T \end{cases} \tag{2.31}$$

2.6 ASSUMPTIONS

VAM2D contains both flow and solute transport models. Major assumptions of the flow model are as follows:

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

Major assumptions of the 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 isotherm and a first order decay constant.
- Chained decay reactions are regarded as irreversible.

2.7 LIMITATIONS

- In performing a variably saturated flow analysis, the code handles only single-phase flow (i.e., water) and ignores the flow of a second phase (i.e., air or other nonaqueous phase) which, in some instances, can be significant.
- Flow and transport in fractures are not taken into account.
- The code does not take into account kinetic sorption effects and/or reversible chemical reactions which, in some instances, can be important.

2.8 INPUT DATA

Input data 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

- Horizontal component of saturated hydraulic conductivity, K_h (LT^{-1})
- Vertical component of saturated hydraulic conductivity, K_v (LT^{-1})
- Cross component of saturated hydraulic conductivity, K_{hv} , if the coordinate system does not coincide with the principal axes of anisotropy (LT^{-1})
- Specific storage, S_s (L^{-1})
- Saturated water content, θ_s

(3) Constitutive Relationships for Variably Saturated Flow

- Parameter n of the Brooks-Corey relation (2.8a).
- Air-entry pressure head, ψ_a (L)
- Parameters α , β and γ of the van Genuchten relations (2.8b) and (2.9) (α has dimensions of L^{-1}).
- Parameters describing anisotropy of relative conductivity.

(4) Initial and Boundary Conditions

- Initial distribution of pressure head, ψ_o (L)
- Prescribed values of pressure head, $\bar{\psi}$ (L)
- Prescribed values of nodal fluid flux, Q (Q has dimensions of L^2T^{-1} for a cross-sectional simulation and L^3T^{-1} for an axisymmetric simulation).

Input data 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)
- Free water molecular diffusion coefficient, D_m (L^2T^{-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^3M^{-1})

(4) Darcy velocity components of the fluid phase considered, v_1 and v_2 (LT^{-1})

(5) Saturation of the fluid phase considered, S_w

(6) Initial and boundary conditions

- Initial distribution of concentration, c_0 (ML^{-3})
- Prescribed values of concentration, c (ML^{-3})
- Prescribed values of solute flux at boundary nodes, q_c (q_c has dimensions of $ML^{-1}T^{-1}$ and MT^{-1}) for cross-sectional and axisymmetric analyses, respectively
- Fluid fluxes at boundary nodes
- Location of potential seepage faces, if any

2.9 OUTPUT

The primary output from the flow model of VAM2D includes nodal values (at user-selected time levels) of pressure head and element centroidal values of Darcy velocity components and water-phase saturation at various time levels. VAM2D allows the user to select a fluid volumetric mass 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, VAM2D also provides the main link of the two models by writing the linking information on FORTRAN Unit 9 (binary format). This information includes computed element centroidal values of Darcy velocities and fluid saturation, nodal fluid storage terms, and boundary nodal flux values. A restart option for the flow model is provided in the code. This is facilitated by writing the nodal values of pressure head computed at the final time step of the current run on FORTRAN Unit 8.

The primary output of the transport model of VAM2D includes nodal values (at user-selected time levels) of solute concentration. VAM2D also allows the user to select a 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 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 velocity backup files for transport simulations. In the sequential simulation approach, the flow problem is solved for the entire time period of simulation. In order to solve the associated transport problem after running the flow problem, the user should select the 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.

VAM2D, finally, can create two optional auxiliary output files (FORTRAN Units 10 and 11) which contain nodal values of the various variables of interest, in a general x-y-z column format, to facilitate the interfacing with commonly used plotting and contouring

software. Output unit 10 contains the nodal coordinates and corresponding nodal values of pressure head and/or concentration(s). For a flow run, output unit 11 contains the element centroidal coordinates, plus values of the quantities that are defined at the element centroids, i.e., water saturation, water content, and Darcy velocity components.

3 NUMERICAL SOLUTION TECHNIQUES

3.1 GENERAL

In this chapter, numerical techniques for approximating the variably saturated flow equation and the non-conservative solute transport equation are described. The flow equation is treated using the Galerkin finite element method. The non-linearity is treated using the Picard and Newton-Raphson iterative techniques.

The transport equation is treated using the upstream-weighted finite element method designed to circumvent numerical oscillations. For both flow and transport problems, spatial discretization is performed using simple rectangular or orthogonal curvilinear elements. The elements may be oriented in an arbitrary manner in the flow domain. Element matrices are computed using highly efficient influence coefficient matrix formulas (Huyakorn et al., 1984, 1985). The systems of algebraic equations resulting from the finite element approximations of the flow and transport equations can be solved in a standard manner using direct (banded matrix) solvers for symmetric and asymmetric matrices, respectively.

3.2 NUMERICAL TECHNIQUES FOR VARIABLY SATURATED FLOW

3.2.1 Galerkin Formulation

Equation (2.3) is solved by the Galerkin finite element method. In the Galerkin procedure, the pressure head function is represented by a trial function of the form

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

where $N_J(x_i)$ and $\psi_J(t)$ 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

$$\int_R K_{ij} k_{rw} \frac{\partial N_I}{\partial x_i} \frac{\partial N_J}{\partial x_j} \psi_J dR + \int_R K_{ij} k_{rw} \frac{\partial N_I}{\partial x_i} e_j dR$$

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

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

$$A_{IJ} \psi_J + B_{IJ} \frac{d\psi_J}{dt} = F_{IJ} \quad , \quad I = 1, 2, \dots, n \tag{3.3}$$

where

$$A_{IJ} = \sum_e \int_{R^e} K_{ij} k_{rw} \frac{\partial N_I}{\partial x_i} \frac{\partial N_J}{\partial x_j} dR \tag{3.4a}$$

$$B_{IJ} = \sum_e \int_{R^e} \eta N_I N_J dR \tag{3.4b}$$

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

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 VAM2D, linear rectangular or orthogonal curvilinear elements are used. For such elements, the element matrices can be evaluated efficiently using influence coefficient formulas given in Huyakorn et al. (1984). When a curvilinear model grid is used, the

elements are treated as slightly deformed rectangular elements. This procedure yields accurate results provided the deviations from a rectangular grid are not too severe.

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 implicit finite difference approximations. Two alternative nonlinear treatment procedures are provided in VAM2D. 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 an asymmetric coefficient matrix. Both schemes are presented briefly in this section.

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

$$\begin{aligned} & \omega A_{IJ}^{k+\omega} \psi_J^{k+1} + (1-\omega) A_{IJ}^{k+\omega} \psi_J^k \\ & + \frac{B_{IJ}^{k+\omega}}{\Delta t_k} (\psi_J^{k+1} - \psi_J^k) = F_I^{k+\omega}, \quad I = 1, 2, \dots, n \end{aligned} \quad (3.5)$$

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 an implicit time-stepping scheme, the value of ω must be equal to or greater than 0.5.

Equation (3.5) is now rearranged in the form

$$\left(\omega A_{IJ}^{k+\omega} + \frac{B_{IJ}^{k+\omega}}{\Delta t_k} \right) \psi_J^{k+1} = F_I^{k+\omega} + (\omega-1) A_{IJ}^{k+\omega} \psi_J^k + \frac{B_{IJ}^{k+\omega}}{\Delta t_k} \psi_J^k \quad (3.6)$$

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. For each iteration the most recent nodal values $\psi_j^{k+\omega}$, determined from $\psi_j^{k+\omega} = (1-\omega)\psi_j^k + \omega\psi_j^{k+1}$, are used to calculate coefficient matrices and the right-hand-side vector. For variably saturated flow simulations, the time weighting coefficient ω is always set to 1.0, i.e., a backward difference time stepping scheme is used. The use of 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:

$$\begin{aligned} G_I &\equiv A_{IJ} \psi_J^{k+1} + B'_{IJ} (\psi_J^{k+1} - \psi_J^k) / \Delta t_k \\ + E_I (S_{wJ}^{k+1} - S_{wJ}^k) / \Delta t &= 0, \quad I=1,2,\dots,n \end{aligned} \quad (3.7)$$

where G_I is the non-linear (vector array) function of the nodal head values, and B'_{IJ} and E_I are defined as

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

$$E_I = \int_R \phi N_I dR \quad (3.8b)$$

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.

The mass lumping scheme implemented in VAM2D is based on an analysis by Milly (1985). Milly (1985) has shown that the formulation of the storage matrix $[B]$, in conjunction with the manner in which the soil moisture capacity $C = d\theta/d\psi$ is evaluated, can have a large effect on the mass balance accuracy of a variably saturated flow simulation. Provided this is done in an appropriate and consistent manner it is possible to obtain a mass-conserving solution even when steep moisture gradients are present. Lumping of the storage matrix is generally recommended with VAM2D since it not only speeds up numerical convergence, but also reduces mass balance errors.

In VAM2D, several convergence enhancement features have been implemented 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

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

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

$$\psi_J^{k+1} = (1 - \gamma) \psi_J^r + \gamma \psi_J^{r+1} \quad (3.13)$$

where γ is an underrelaxation factor ($0 < \gamma < 1$), and ψ_J^r 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 under-relaxation 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:

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

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 ($e_r = \text{Max}_i |\psi_i^r - \psi_i^{r-1}|$).

The third convergence enhancement feature is the (optional) 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.

In addition to the mentioned convergence features, VAM2D utilizes automatic time step reduction and marching procedure to handle convergence difficulties. The procedure is described in Section 5.6.2.

3.2.3 Treatment of Evaporation and Infiltration Boundary Conditions

An iterative procedure is used to handle evaporation and infiltration boundary conditions. This procedure is adapted from that used by Neuman et al. (1974). It is described as follows:

- During the first iteration in each time step, treat all surface nodes subjected to infiltration or evaporation as prescribed flux nodes. Assign to these nodes flux values that correspond to a certain fraction of $|E^*|$.
- Check whether computed pressure head values, ψ_I , satisfy the head value constraint ($\psi_L \leq \psi_I \leq 0$).
- For the nodes satisfying the head constraint, update the prescribed flux values by reassigning f_I^{r+1} , the fraction of the maximum potential infiltration (or evaporation) rate to be applied at iteration $r+1$. The value $f_I^{r+1} = f^*$ for $r = 0$, $f_I^{r+1} = f_I^r + (f^*)^{1/(r+1)} \leq 1$ for $r \geq 1$, where f^* is a preset initial value of fraction of the maximum potential infiltration (or evaporation) rate assigned to the node. Note that $0 < f^* \leq 1$.
- For the nodes at which ψ_I does not satisfy the head constraint, alter the boundary conditions from prescribed flux to prescribed head. For the next iteration set the head values ψ_I to ψ_L for evaporation, and to zero for infiltration. Compute the flux values and check whether they satisfy the flux constraint. If, at any stage of the computation, the computed flux at node I exceeds the maximum potential flux, then in the next iteration apply the flux boundary condition to that node and set its nodal flux value equal to the maximum potential flux.
- Repeat the above iterative procedure until convergence is achieved at all nodes in the finite element network.

3.2.4 Treatment of Seepage Faces

For cases involving seepage faces, another type of atmospheric boundary condition known as the "seepage face boundary condition" applies. This type of boundary condition is nonlinear because the seepage face positions are unknown a priori, and must be located by

trial and error. Methods for locating seepage faces can be found in several references (e.g., Rubin, 1968; Neuman et al., 1974; Cooley, 1983). The approach of Neuman et al. (1974) is used here.

The solution procedure starts with an initial position of the seepage face and proceeds to predict the position at the next time level. Within the time step, iterations are performed and, if necessary, the height of the seepage face is adjusted at the end of each iteration. The aim is to satisfy the conditions of zero ψ values on the seepage face, negative ψ values at the nodes above the seepage face, and negative flux (outflow) values at the seepage face nodes. All nodes expected to be part of the seepage face during the course of the simulation are considered. Their boundary conditions may be switched from prescribed zero ψ values to prescribed zero flux values to meet the necessary constraints. To enhance convergence of the solution, the modification of boundary conditions proceeds sequentially from node to node, starting at the saturated end of the seepage face. The iterative process continues until a sufficient degree of convergence is achieved at each node in the finite element network.

3.2.5 Treatment of Water Uptake by Plant Roots

Uptake of water by plant roots is handled by including a root extraction term q^* as part of the sink term on the right-hand side of the flow equation (2.3). The root extraction term, q^* , is represented (Feddes et al., 1974) as

$$q^* = Kk_{rw}(\psi - \psi_r)f_r \quad (3.16)$$

where K is the mean hydraulic conductivity defined as $K = (K_{11} + K_{22} + K_{33})/3$, ψ_r is the pressure head in the plant roots, and f_r is a root effectiveness function.

To simplify the coding, the root zone is discretized into columns of rectangular elements. All elements in the root zone are identified, and plant species numbers are also assigned to individual nodal columns. Note that only the nodes below the soil surface are counted as part of the root zone. The nodes at the soil surface are assumed to be contributing only to direct evaporation and not to root extraction. Data for each plant species must be supplied as input. These data include: wilting pressure head, ψ_w , potential transpiration rate, E_{pl} , and relationship of root effectiveness function versus depth.

Because the rate of water uptake by plant roots depends on atmospheric conditions and conditions underground, it cannot be predicted a priori. Thus iterations must be performed to maximize the total rate of transpiration per unit surface area, E_{pl} , so that the following constraints are satisfied:

$$|E_{pl}| \leq |E_{pl}^*| \quad (3.17a)$$

and

$$\psi_r \geq \psi_w \quad (3.17b)$$

The constrained maximization is achieved using the procedure introduced by Neuman et al. (1974). For each time step, the calculation procedure for each individual nodal root-zone column is outlined as follows:

- Set ψ_r equal to ψ_w .
- Compute integrated nodal values of root extraction flux, Q_I , using current values of pressure head and relative permeability. For the nodes with $Q_I^* > 0$, set $Q_I^* = 0$.
- Compute E_{pl} for the nodal column:

$$E_{pl} = \frac{1}{A_c} \sum_{I=1}^e Q^* \quad (3.18)$$

where n_c is the number of effective nodes in the column, and A_c is the surface area of the column.

- If $|E_{pl}|$ is less than or equal to $|E_{pl}^*|$, use the computed values of Q_I^* in the solution of the system of finite element equations (3.6).
- If $|E_{pl}|$ is greater than $|E_{pl}^*|$, adjust computed values of Q_I^* by a factor of $|E_{pl}^*|/|E_{pl}|$ to make their sum equal to E_{pl}^* . Update the root pressure head by determining its new value from

$$E_{pl} = \frac{1}{A_c} \sum_{I=1}^{n_c} Q_I^* = \frac{1}{A_c} \sum_{I=1}^{n_c} \alpha_I (\psi_I - \psi_r) \quad (3.19)$$

where $\alpha_I = Kk_{rw}f_{rI}$.

- The above process is performed for each vertical nodal column within the root zone. After all components of Q_I^* have been determined, the system of finite element equations (3.6) is solved. Iterations are performed until convergence is obtained.

3.2.6 Treatment of Hysteresis and Anisotropy

To simulate the effect of hysteresis in soil moisture properties in a variably saturated flow simulation, VAM2D incorporates the procedure described by Kool and Parker (1987). This procedure requires that the boundary wetting and drying curves in the $S_w(\psi)$ relation are known. In VAM2D it is assumed that these boundary curves are described by expressions that have the same form as (2.9), but with different parameter values for wetting and drying boundaries. Using superscripts w and d to distinguish between wetting and drying, respectively, the boundary $S_w(\psi)$ curves are described by the following relationships

$$\frac{S_w^w - S_{wr}}{1 - S_{wr}} = \begin{cases} \frac{1}{[1 + (\alpha^w |\psi - \psi_a|)^{\beta^w}]^{\gamma^w}} & \psi < \psi_a \\ 1 & \psi \geq \psi_a \end{cases} \quad (3.20)$$

$$\frac{S_w^d - S_{wr}}{1 - S_{wr}} = \begin{cases} \frac{1}{[1 + (\alpha^d |\psi - \psi_a|)^{\beta^d}]^{\gamma^d}} & \psi < \psi_a \\ 1 & \psi \geq \psi_a \end{cases} \quad (3.21)$$

In equation (3.20) S_{ws} represents the maximum saturation value upon rewetting of an initially air-dry soil. If no air-entrapment occurs, $S_{ws} = 1.0$. However, if air-entrapment occurs, S_{ws} will be less than one. Parameters α , β and γ are the van Genuchten curve shape parameters, with different values for wetting and drying. Note that α^w cannot be less than α^d , i.e.

$$\alpha^w \geq \alpha^d$$

Often, the following simplifications can be used (Kool and Parker, 1987)

$$\beta^w = \beta^d = \beta$$

$$\gamma^w = \gamma^d = 1 - 1/\beta$$

With these simplifications, only five parameters are required to characterize the hysteretic saturation-pressure head relation. The parameters are the porosity, ϕ , residual saturation, S_{wr} , and shape parameters α^w , α^d and β . Lacking data, one may use $\alpha^w = 2\alpha^d$ as a first approximation (Kool and Parker, 1987). A typical hysteretic $S_w(\psi)$ relation is shown in Figure 3.1. This figure illustrates the correspondence of the parameters in (3.20) and (3.21) to the boundary wetting and drying curves.

In a hysteretic flow simulation, VAM2D automatically computes scanning curves in the $S_w(\psi)$ relation to determine the appropriate saturation path for every element in the modeled domain when reversals from wetting to drying, or vice-versa occur. This is achieved by defining "pseudo" values of the residual and saturated values of S_w . In the simulation, these pseudo-values are substituted into Eqs. (3.20) and (3.21). This has the effect of scaling the boundary wetting and drying curves to make them pass through the reversal points. For a reversal from wetting to drying, the nominal value of 1.0 for S_w at saturation is replaced by

$$S'_{ss} = \frac{S_w^{rev} - S_{wr} [1 - S_e^d(\psi^{rev})]}{S_e^d(\psi^{rev})} \quad (3.22)$$

where S_w^{rev} and ψ^{rev} are the saturation and pressure head at the reversal point, respectively and $S_e^d(\psi^{rev})$ is the effective drying saturation given by the left hand side of (3.21) for $\psi = \psi^{rev}$. Analogously, for a reversal from drying to wetting, a pseudo-value for S_{wr} is used, which is given by

$$S'_{wr} = \frac{S_w^{rev} - S_e^w(\psi^{rev})}{1 - S_e^w(\psi^{rev})} \quad (3.23)$$

where S_e^w is the effective wetting saturation corresponding to the left hand side of (3.20). The hysteresis subroutine in VAM2D checks whether each element is wetting or drying and computes the appropriate values of S'_{ss} and S'_{wr} for each element. This is achieved by means

Figure 3.1. Example of hysteretic $S_w(\psi)$ relation showing the boundary wetting and drying curves.

of an index variable, κ_i , which is set to $\kappa_i = +1$ if the i -th element is wetting and $\kappa_i = -1$ if the i -th element is drying. At the end of every time step a check is made for every element to determine whether a reversal in the saturation path has occurred. A reversal occurs if

$$\frac{\bar{\psi}_i^{t-\Delta t} - \bar{\psi}_i^t}{\kappa_i} > \delta_\psi \quad (3.24)$$

where δ_ψ is the pressure head iteration convergence tolerance, and $\bar{\psi}_i$ is the average nodal pressure head for the i -th element

$$\bar{\psi}_i = \frac{1}{n_i} \sum_{j=1}^{n_i} \psi_{ij} \quad (3.25)$$

with n_i the number of nodes for the element. When a reversal occurs, the code determines the new scanning curve for the element which is subsequently used to calculate $S_w(\psi)$. An example of such scanning curves is shown in Figure 3.2. In this example the boundary hysteresis loop is closed at saturation, i.e., $S_{ws} = 1.0$. The figure shows a primary wetting scanning curve (1) and a secondary drying scanning curve (2). In order to completely specify the initial conditions for a hysteretic simulation, the user must specify not only the initial nodal values of ψ , but also the initial saturation values for each element, and whether the element is initially wetting or drying.

VAM2D can further simulate the effect of saturation dependent anisotropy on unsaturated flow by using Eq. (2.12) to evaluate anisotropy as a function of pressure head. This requires input values of the variables σ_f^2 , σ_a^2 , μ and ω . The parameter $\bar{a}$ can be treated either as an input variable or be evaluated by VAM2D as the derivative of the $\ln[k_{rw}(\psi)]$ relation. When the latter option is used with either (2.8a) or (2.8b) to describe the $k_r(S_w)$ relation, the value of $\bar{a}$ will tend to decrease with decreasing saturation. This will magnify the predicted anisotropy compared to the case of a user-specified, constant value for $\bar{a}$. In order to obtain an operational algorithm, two additional criteria were implemented:

First, a maximum bound must be imposed on the anisotropy ratio. Inspection of (2.12) shows that otherwise the computed anisotropy ratio will easily become unrealistically large, even for moderate values of ψ . The upper bound, $r_{\max}$, for $r(\psi)$ is a user-specified value in VAM2D. A value of $r_{\max} = 10^7$ has been found to give satisfactory results in many cases. Secondly, Eq. (2.12) gives the conductivity ratio, but not the actual values of conductivities parallel and perpendicular to stratification. In order to obtain the desired, monotonically decreasing $k_{rw}(\psi)$ relations, VAM2D uses an empirical logarithmic

Figure 3.2. Typical scanning curves produced by the hysteresis model in VAM2D. Curve (1) denotes primary wetting scanning curve, curve (2) denotes secondary drying scanning curve.

interpolation procedure to ensure that both $(Kk_{rw})_{11}$ and $(Kk_{rw})_{22}$ decrease with decreasing pressure head and that the correct anisotropy ratio is maintained for any ψ value. An example anisotropic $k_{rw}(\psi)$ relation as modeled by VAM2D is shown in Figure 3.3. This figure shows relative conductivity as a function of soil water pressure head. The solid curve represents the isotropic case in which conductivity is given by (2.8b) and (2.9). The dashed lines represent the anisotropic case with anisotropy ratio computed from (2.12). The following anisotropy parameters were used here: $\sigma_f^2 = 0.82$, $\sigma_a^2 = 0.0005$, $\mu = 40$ cm and $\omega = 0.0$. The figure clearly illustrates the dramatic effect of tension (pressure head) variations on the magnitude of anisotropy.

3.2.7 Total Head Formulation

With this option, the flow equation (3.3) is solved for the total piezometric (hydraulic) head, $h = \psi + z$ (where z is the elevation above datum), at any location in the domain. Hence, during solution, the gravity term (the first term on the right hand side of (3.4c)) is neglected, since it is included in the definition of the total head. This gravity term is subtracted from the total head, however, whenever calculations involve the pressure head (e.g., in the moisture retention function (2.9)). This has the advantage that gradients of the gravity term do not have to be calculated. This is particularly useful in a curvilinear grid system with irregular nodal coordinates. Consequently, the total head formulation, rather than the pressure head formulation, should be employed when using the curvilinear grid option.

3.3 NUMERICAL TECHNIQUE FOR SOLUTE TRANSPORT

3.3.1 Upstream Weighted Residual Formulation

For the contaminant transport simulation, VAM2D solves (2.20) for single species transport or (2.23) for multi-species transport using an upstream weighted residual finite element method. To illustrate the application of the technique, consider equation (2.20) and a trial solution for concentration be written in the form:

$$c(x_i, t) = N_J(x_i) c_J(t) \quad (3.26)$$

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

Figure 3.3. Example of anisotropic $k_{rw}(\psi)$ relation as modeled by VAM2D.

functions to weight the remaining mass accumulation term. Application of this procedure to (2.20) yields

$$\begin{aligned} & \int_R W_I \left[\frac{\partial}{\partial x_i} (D_{ij} \frac{\partial c}{\partial x_j}) - v_i \frac{\partial c}{\partial x_i} \right] dR \\ & - \int_R N_I \left[\phi S_w R \left(\frac{\partial c}{\partial t} + \lambda c \right) + q(c - c^*) \right] dR = 0 \end{aligned} \quad (3.27)$$

where W_I are the upstream weighting functions.

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

$$\begin{aligned} & \int_R (D_{ij} \frac{\partial W_I}{\partial x_i} \frac{\partial N_J}{\partial x_j} + v_I W_I \frac{\partial N_J}{\partial x_i}) c_J dR \\ & + \int_R \phi S_w R N_I N_J \left(\frac{dc_J}{dt} + \lambda c_J \right) dR + \int_R N_I q (c^* - N_J c_J) dR \\ & - \int_R W_I (D_{ij} \frac{\partial c_J}{\partial x_j}) n_i dB = 0 \end{aligned} \quad (3.28)$$

Equation 3.28 can be expressed in the form

$$(E_{IJ} + B_{IJ}^*) c_J + \tilde{B}_{IJ} \frac{dc_J}{dt} = \tilde{F}_I \quad (3.29)$$

where

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

$$E_{ij} = \int_R (D_{ij} \frac{\partial W_I}{\partial x_i} \frac{\partial N_J}{\partial x_j} + v_i W_I \frac{\partial N_J}{\partial x_i}) dR$$

$$\tilde{B}_{IJ} = \int_R (\phi S_w R) N_I N_J dR$$

$$B_{IJ}^* = \int_R (\lambda \phi S_w R) N_I N_J dR$$

Once all of the element matrices have been computed and assembled into global matrices, the system of ordinary differential equations (3.29) can be integrated with respect to time. This leads to the following system of algebraic equations

$$\begin{aligned} (\omega (E_{IJ} + B_{IJ}^*) + \frac{\tilde{B}_{IJ}}{\Delta t_k}) c_J^{K+1} &= (\omega - 1) (E_{IJ} + B_{IJ}^*) c_J^k + \frac{\tilde{B}_{IJ}}{\Delta t_k} c_J^k \\ &+ \omega \tilde{F}_I^{k+1} + (1 - \omega) \tilde{F}_I^k \end{aligned} \quad (3.30)$$

where ω is the time weighting factor.

Equation 3.30 can be rearranged in the form

$$G_{IJ} c_J^{k+1} = R_I^{k+1} \quad (3.31)$$

where

$$R_I^{k+1} = (\omega - 1) (E_{IJ} + B_{IJ}^*) c_J^k + \frac{\tilde{B}_{IJ}}{\Delta t_k} c + \omega \tilde{F}_I^{k+1} + (1 - \omega) \tilde{F}_I^k \quad (3.32a)$$

and

$$G_{IJ} = \omega (E_{IJ} + B_{IJ}^*) + \tilde{B}_{IJ} / \Delta t_k \quad (3.32b)$$

To obtain a second-order accuracy in time approximation, ω is chosen to be 0.5 thus yielding the Crank-Nicolson time stepping scheme. Equation (3.31) represents a system of linear algebraic equations with an asymmetric banded coefficient matrix. Its solution is achieved by using a direct banded matrix solver.

3.3.2 Treatment of Boundary Conditions for Single Component Transport

The first-type boundary condition (2.22b) 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 equality assumption is adopted.

The second-type boundary condition (2.22c) 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 fluid 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 (2.22d) 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 (2.22d) 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 (2.22d) then reduces to that of (2.22c) 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.

3.3.3 Treatment of Boundary Conditions for Chained Decay Transport

The three boundary conditions (2.22a) - (2.22c) for chained decay transport are treated in a similar manner to those of single-component transport. In the case of a decaying source, the prescribe source concentrations of solute mass fluxes released from the source are computed using the general analytical solution of the Bateman equation (2.29).

3.4 MASS BALANCE COMPUTATION PROCEDURE

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 2.1 and applying Green's theorem to the spatial derivative terms. Thus, one obtains

$$\int_B k_{ij} k_{rw} \left(\frac{\partial \psi}{\partial x_j} + e_j \right) dB - \int_R \eta \frac{\partial \psi}{\partial t} dR + \int_R q dR = 0 \quad (3.33)$$

where

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

It should be noted that the first integral in Equation 3.33 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 3.33, the right hand side will be zero. However, if an approximate finite element solution ψ is substituted,

the right-hand side of (3.33) will be non-zero, and will correspond to an error in material balance, $\dot{e}_v$

$$\dot{e}_v = - \int_B v_I n_i dB - \int_R \eta \frac{\partial \psi}{\partial t} dR + \int_R q dR \quad (3.34)$$

where

$$q = \sum_{I'=1}^{n_w} Q_{I'} \delta(\bar{x} - \bar{x}_{I'})$$

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

n_w is the number of source/sink nodes and $Q_{I'}$ is the volumetric fluid injection rate. Next, we make use of the following properties of the basis functions:

$$\sum_{I^*=1}^{n_B} N_{I^*}^*(\bar{x}^*) = 1 \text{ for all } \bar{x}^* \text{ on } B \quad (3.35)$$

and

$$\sum_{I=1}^n N_I(x) = 1 \text{ for all } x \text{ on } R \quad (3.36)$$

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

Combining Equations 3.34-3.36 yields

$$\begin{aligned} \dot{e}_v = & \sum_{I^*=1}^{n_B} - \int_B N_{I^*} v_i n_i dB - \sum_{I=1}^n \left(\int_R \eta N_I N_J \frac{d\psi_J}{dt} dR \right) \\ & + \sum_{I'=1}^{n_w} Q_{I'} \end{aligned} \quad (3.37)$$

Equation 3.37 can be written in the form

$$\dot{e}_v = \sum_{I^*=1}^{n_B} -f_{I^*}^B - \sum_{I=1}^n f_I^S - \sum_{I'=1}^{n_w} f_{I'}^W \quad (3.38)$$

where

$$\begin{aligned} f_{I^*}^B &= \int_B N_{I^*} v_i n_i dB \\ f_I^S &= \int_R \eta N_I N_J \frac{d\psi_J}{dt} dR, \quad f_{I'}^W = Q_{I'} \end{aligned}$$

The storage and sink and source terms in Equation 3.38 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 to obtain $f_{I^*}^B$.

After all the terms in 3.34 have been computed, the error in the rate of material balance, $\dot{e}_v$, can be determined. For each time level, the cumulative material balance error, E_v^t , is evaluated from

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

$$||E_v|| = |E_v| / \left[\sum_{I^*=1}^{n_B} |f_{I^*}| + \sum_{I=1}^n |f_I^I| + \sum_{I'=1}^{n_w} |f_{I'}^w| \right] \quad (3.40)$$

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 (2.20) is obtained

$$\begin{aligned} \int_B (D_{ij} \frac{\partial c}{\partial x_j} - v_i c) n_i dB - \int_R \left(\frac{\partial}{\partial t} (\phi S_w R c) + \phi \lambda S_w R c \right) dR \\ + \sum_{I'=1}^{n_w} Q_{I'} c_{I'}^* = 0 \end{aligned} \quad (3.41)$$

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

$$\begin{aligned} \dot{e}_M = \sum_{I^*=1}^{n_B} \int_B N_{I^*} (D_{ij} \frac{\partial c}{\partial x_j} - v_i c) n_i dB \\ - \sum_{I=1}^n \int_R \phi S_w R N_I N_J \left(\frac{dc_J}{dt} + \lambda c_J \right) dR + \sum_{I'=1}^{n_w} Q_{I'} c_{I'}^* \\ - \sum_{I=1}^n \int_R N_I N_L c_L \eta N_J \frac{d\psi_J}{dt} dR \end{aligned} \quad (3.42)$$

which can be expressed in the form

$$\dot{e}_M = - \sum_{I^*=1}^{n_B} F_{I^*}^B - \sum_{I=1}^n f_I^S + \sum_{I'=1}^{n_w} F_{I'}^w \quad (3.43)$$

where

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

$$F_I^s = \int_R \phi S_w R N_I N_J (\frac{dc_J}{dt} + \lambda c_J) dR + \sum_{l=1}^n \int_R N_L c_L (\eta N_I N_J \frac{d\psi_J}{dt}) dt$$

$$F_I^w = Q_{I'} c_{I'}^*$$

Except for the boundary integral term, all other terms in Equation 3.42 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

$$(v_i c - D_{ij} \frac{\partial c}{\partial x_j}) n_i = q_c^T \quad (3.44)$$

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

$$F_{I^*}^B = \int_B N_{I^*} q^T dB \quad (3.45)$$

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

$$-D_{ij} \frac{\partial c}{\partial x_j} n_i = q_c^D \quad (3.46)$$

and the outward advective flux is obtainable from

$$v_i n_i c = q N_J c_J \quad (3.47)$$

where q is the outward normal fluid flux distribution. Equations 3.46 and 3.47 are combined with Equation 3.45 to yield

$$\begin{aligned}
F_{I^*}^B &= \int_B N_{I^*} (q N_J c_J + q_c^D) dB \\
&\approx c_{I^*} \int_B N_{I^*} q dB + \int_B N_{I^*} q_c^D dB
\end{aligned}
\tag{3.48}$$

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 $Q_c^{DI^*}$ has been computed the total boundary nodal flux is obtainable from

$$F_{I^*}^B \approx c_{I^*} \int_B N_{I^*} q dB + Q_{cI^*}^D \tag{3.49}$$

Finally, when all the various material flux terms have been computed, the error in the rate of material balance, $\dot{e}_M$ can be determined from Equation 3.43. In practice, the cumulative mass balance error at a current time level, E_M^t should also be computed. It is given by

$$E_M^t = \sum_{\ell=1}^k (\dot{e}_M \Delta t_\ell) \tag{3.50}$$

Both E_M^t and its normalized form $\bar{E}_M^t$, are used as indicators of the global accuracy of the numerical solution of the transport equation. For convenience, we define $\bar{E}_M^t$ as

$$\bar{E}_M^t = \sum_{\ell=1}^k \{ (\dot{e}_M \Delta t_\ell) / (\sum_{\ell=1}^n F_I^s) \} \tag{3.51}$$

4 EXAMPLE VERIFICATION AND APPLICATION PROBLEMS

4.1 GENERAL

Two sets of test problems were used for verification of numerical schemes and demonstration of major capabilities of the VAM2D code. Specific purposes of the example problems presented in this chapter are described below.

- Simulation of water flow under variably saturated (or saturated-unsaturated) conditions
- Simulation of single and multiple component transport
- Coupled simulation of flow and transport problems with various types of boundary conditions
- Simulation of a laboratory column experiment on hysteric flow
- Simulation of an intermediate-scale field experiment on solute transport in a Caisson
- Verification of the VAM2D code against analytical solutions and other finite element variably saturated flow and transport codes (UNSAT2, FEMWATER and FEMWASTE, and VADOFT)
- Demonstration of the ability of VAM2D to cope with highly nonlinear conditions

The first problem set comprises seven transient and steady-state flow problems with different features of boundary conditions and varying degree of nonlinearity. These problems are as follows:

- Horizontal flow in a soil slab
- Transient evaporation and infiltration in a soil column
- Transient hysteretic flow in a soil column
- Transient two-dimensional flow in an unconfined aquifer adjacent to a landfill
- Transient two-dimensional flow in a root zone

- Steady-state two-dimensional flow beneath a landfill
- Transient vadose-zone infiltration under initially dry soil conditions.

The second problem set comprises seven transient transport problems. Three of these problems are associated with three of the seven flow problems just mentioned. The transport problems considered are listed as follows:

- One-dimensional horizontal transport in a soil slab
- Two-dimensional transport in a soil slab
- One-dimensional transport of two three-member chains of radionuclides
- Two-dimensional transport in uniform groundwater flow
- Transient two-dimensional transport in a root zone
- Leachate migration from a sanitary landfill
- Simulation of solute transport in a Caisson experiment.

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

4.2 VARIABLELY SATURATED FLOW PROBLEMS

4.2.1 One-Dimensional Flow in a Horizontal 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 case in which there is no gravity effect. The problem is depicted schematically in Figure 4.1. As illustrated, a slab of soil 20 cm long has an initial pressure head of -83.33 cm. Wetting occurs at the left boundary ($x = 0$) where the pressure head is increased to 0.0 and maintained constant. The pressure head at the right boundary ($x = 20$ cm) is kept constant at -83.33 cm. For convenience, the soil was assumed to be homogeneous and isotropic with a saturated hydraulic conductivity of $1 \text{ cm} \cdot \text{d}^{-1}$ and porosity of 0.45. The soil moisture characteristics used in the simulation are

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

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

and

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

where $S_{wr} = 0.3333$ and $\psi_a = 0.0$ cm. The selected, linear, relative permeability function corresponds to the Brooks-Corey equation with $n = 1$. The selected water saturation function corresponds to the van Genuchten equation with $\alpha = -0.01 \text{ cm}^{-1}$, $\beta = 1$ and $\gamma = -1$.

Values of the saturated hydraulic conductivity and the porosity employed in the simulation are also depicted in Figure 4.1. Numerical solutions were obtained using a uniform mesh spacing, with $\Delta x = 1$ cm, $\Delta y = 4$ cm and a constant time increment, $\Delta t = 0.01$ days. In Figure 4.2, the pressure head profiles computed by VAM2D are compared with those computed by 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. For reference purposes, a tabulation of the values of inflow rate versus time obtained from VAM2D and UNSAT2 is provided in Table 4.1.

4.2.2 Transient Evaporation and Infiltration in a Soil Column

This problem concerns one-dimensional vertical flow in an unsaturated zone above a water table. It is selected to test the implementation of the Galerkin finite element formulation, the Picard iterative procedure, as well as the schemes for handling nonlinear atmospheric boundary conditions due to infiltration and evaporation. Two cases were simulated: case 1 involves infiltration and evaporation, and case 2 involves a no flow boundary condition on the top soil surface.

For case 1, the flow region representing a soil column is shown in Figure 4.3 together with the two-dimensional coordinate system used in the simulation. The soil properties are given in Table 4.2.

The flow region was discretized using a rectangular grid consisting of 40 elements and 82 nodes. A constant nodal spacing was used along each coordinate axis. The spacings in the x and y directions were $\Delta x = 50$ cm and $\Delta y = 5$ cm, respectively. Initially, the soil was assumed to be dry having a water phase saturation of 0.35. The bottom of the flow region corresponds to the water table where a zero pressure head was prescribed. The soil surface was then subjected to infiltration (Case 1a) for the duration of 10 d. The maximum potential infiltration flux was prescribed as $5 \text{ cm} \cdot \text{d}^{-1}$. The simulation of the response to infiltration was performed for 18 time steps. The time stepping was started with an initial

Figure 4.2. Pressure head distributions along the base and the top of the flow region.

Figure 4.3. Geometry and boundary conditions used in the simulation of case 1 of the soil column problem.

Table 4.1. Net inflow rate versus time computed by VAM2D and UNSAT2 for test problem 4.2.1

Time (days)	Inflow rate (cm ³ /day)	
	VAM2D	UNSAT2
0.01	39.09	21.79
0.02	18.63	16.65
0.03	14.06	13.39
0.04	11.74	11.44
0.05	10.28	10.13
0.06	9.262	9.177
0.07	8.495	8.446
0.08	7.892	7.864
0.09	7.402	7.386
0.10	6.993	6.983
0.11	6.645	6.637
0.12	6.344	6.335
0.13	6.080	6.068
0.14	5.846	5.827
0.15	5.636	5.610

Table 4.2. Soil Properties Used in the Simulation Case 1 of the Soil Column Problem.

Parameter	Value
Saturated hydraulic conductivity, K	$10 \text{ cm} \cdot \text{d}^{-1}$
Porosity, ϕ	0.45
Residual water phase saturation, S_{wr}	0.333
Air entry value, ψ_a	0.0 cm
Maximum potential surface flux, $ E_s^* $	$5 \text{ cm} \cdot \text{d}^{-1}$
Minimum allowable pressure head at soil surface, ψ_L	-90 cm

Constitutive relations:

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

$$(\psi - \psi_a) / (\psi_r - \psi_a) = (1 - S_w) / (1 - S_{wr})$$

where $\psi_r = -100 \text{ cm}$.

step of 0.1 d and was enlarged using a multiplier of 1.2 to a maximum value of 1 d. Computed pressure head distributions (Case 1a) are presented in Figure 4.4 for five time values. Also included in this figure are the numerical results from the UNSAT2 code, which illustrate reasonably good agreement between the numerical solutions from VAM2D and UNSAT2.

The soil surface was next subjected to evaporation (Case 1b). The potential evaporation flux was specified as $5 \text{ cm} \cdot \text{d}^{-1}$ for a second time period of 10 d. It took 22 time steps to cover the 10 d of evaporation. The time stepping was started with an initial step of 0.05 d and was enlarged using a multiplier of 1.2 to a maximum value of 1 d. Computed pressure head distributions (Case 1b) are presented in Figure 4.5 for typical time values. The numerical results from VAM2D are in excellent agreement with the results from UNSAT2.

Case 2 concerns one-dimensional vertical flow in an unsaturated zone above the water table. It is selected to test the implementation of the Galerkin finite element formulations, the Picard iterative scheme, as well as different schemes for handling mass lumping of the storage matrix. The problem is depicted schematically in Figure 4.6. A vertical column of soil 20 cm long was initially subjected to a hydrostatic pressure head distribution. At later time values the pressure head at the lower end was maintained at zero value. A no-flow boundary condition was applied at the top end. Values of the saturated hydraulic conductivity and the porosity as well as the constitutive relationships were the same as those used in case 1. The simulation was performed for 15 time steps using a constant value of $\Delta t = 0.01 \text{ d}$. Two schemes were used to obtain numerical solutions; mass lumping of the storage matrix (scheme 1) and no lumping (scheme 2). Results for $t = 0, 0.01, 0.06, 0.11,$ and 0.15 d are plotted in Figures 4.7 and 4.8. The pressure head and saturation profiles computed by VAM2D and UNSAT2 are in good agreement. Note that the predicted position of water table and water saturation for scheme 1 is slightly ahead of scheme 2 for early time steps. This is probably due to the mass lumping of the element storage matrix.

4.2.3 Transient Hysteretic Flow in a Soil Column

This problem involves transient, one-dimensional hysteretic flow in a vertical soil column subject to drainage and infiltration. The problem simulated is the slow drainage-rewet experiment described by Gillham et al. (1979). In this example the soil moisture relationship (Figure 4.9) exhibits considerable hysteresis. The data points in Figure 4.9 represent the experimental data, while the solid lines were obtained by performing a least-squares fit of van Genuchten equation to this data. The $k_r(S_w)$ relationship of the material (Dune Sand) is given by the following relationship

$$k_r = S_w^n$$

Figure 4.4. Pressure head distributions during infiltration for case 1a.

Figure 4.5. Pressure head distributions for the evaporation case 1b (time values from left to right = 0, 0.05, 0.11, 0.27, 0.65, 1.98, 4.37, and 10.0 d).

Figure 4.6. Geometry and boundary conditions used in the simulation of case 2.

Figure 4.7. Pressure head distributions for case 2.

Figure 4.8. Water phase saturation profiles for case 2.

Figure 4.9. Boundary wetting and drying $S_w(\psi)$ curves of the Dune Sand used in problem 4.2.3. Data points represent measured data of Gillham et al. (1979). The curves represent fitted $S_w(\psi)$ functions.

Parameter values for the unsaturated flow constitutive relations are given in Table 4.3. The experimental configuration in the experiment of Gillham et al. consisted of an initially saturated, 60 cm tall column. The column was first drained and then rewetted by varying the pressure head at the base of the column. A plot of the controlled bottom boundary pressure head as a function of time is shown in Figure 4.10. The imposed variations in bottom boundary pressure head cause the column to drain (along the boundary drying curve), followed by rewetting (along primary wetting curves) after $t = 60$ minutes. The VAM2D simulation of this experiment is shown in Figure 4.11. The data points in this figure represent measured saturations at $t = 68$ min and $t = 125$ min. Saturation profiles predicted by VAM2D are represented by the solid lines. The dashed curve represents simulation results of Gillham et al. The measured data in Figure 4.11 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 VAM2D simulation results and those of Gillham et al. are in generally good agreement with the measured results and with each other. Some deviations between the codes are apparent though. VAM2D predicts somewhat higher saturations between 10 and 20 cm elevation at $t = 68$ min, and there are also some differences between the two simulations at $t = 125$ min. These differences in saturation profiles are due mainly to differences in the way hysteresis is modeled in the two codes. At the first time value shown, $t = 68$ min, the part of the column below 27 cm elevation has started to rewet, while the upper part of the column is still draining. In the VAM2D simulation, the wetting-drying boundary at this time is predicted to be at 25 cm elevation. At $t = 125$ min, both the measured and simulated results indicate that the entire column is wetting. Allowing for the scatter in the experimental data, Figure 4.11 shows a quite good agreement between observed and simulated saturation profiles.

4.2.4 Transient Two-Dimensional Flow in an Unconfined Aquifer Adjacent to a Landfill

In this example, a transient simulation of saturated-unsaturated flow in a complex groundwater system adjacent to a landfill site is presented. Data used in this simulation was assembled using some general information extracted from Silka et al. (1982). The cross section analyzed is depicted in Figure 4.12. Three distinct layers are considered. The top layer is made of a loam material, whereas the middle and the lower layers are made up of dissected clay and a mixture of clay and till, respectively. The landfill site corresponds to a canal which is presently backfilled with the loam and clay materials. There exists a semipermeable clay cap, extending over 125 m length from the center of the landfill, which corresponds to the right vertical boundary of the flow region. To control the water table position, a tile drain was placed at 100 m from the right vertical boundary. In addition, a pump was also placed in the basement of a building located at a distance of 207.5 m from the right vertical boundary of the landfill. This pump is normally put into operation whenever the water level in the basement lies above the bottom of the basement.

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

Parameter	Value
Porosity, ϕ	0.301
Air entry pressure head, ψ_a	0.0
Wetting saturation, S_{ws}	1.0
Residual saturation, S_{wr}	0.332
Wetting curve parameter, α^w	0.0547 cm ⁻¹
Wetting curve parameter, β^w	4.264
Wetting curve parameter, γ^w	0.765
Drying curve parameter, α^d	0.0302 cm ⁻¹
Drying curve parameter, β^d	8.904
Drying curve parameter, γ^d	0.888
Saturated conductivity, K_s	23.56 cm/hr
Exponent, n	5.509

Figure 4.10. A plot of the controlled pressure head at the bottom of the soil column versus time for problem 4.2.3.

Figure 4.11. Comparison of measured and simulated saturation profiles at two time values.

Figure 4.12. Schematic cross-section of the problem of transient flow in an unconfined groundwater system adjacent to a landfill.

The initial condition for this problem corresponds to a static water level 32 m above the base of the clay and till layer. The boundary conditions are as shown in Figure 4.12. Note that the water level in the drain is fixed at 4 m below the base of the desiccated clay layer, and when the pump is in operation, the water level in the basement is fixed at 6 m from the top. Vertical recharge is applied to the top boundary at two different rates, as depicted in Figure 4.12.

The soil material properties used in the simulation are given in Table 4.4. The function of water saturation versus pressure head was taken from van Genuchten et al. (1977), whereas the function of relative permeability versus water saturation was taken from Brooks and Corey (1966) and Mualem (1976). Although the constitutive relations used in this example are not as highly nonlinear as those used in the two previous examples, the present simulation is probably as difficult as the previous simulations. This is because in the present case it is necessary to accommodate sudden and large changes of head values at the drain and the basement boundaries, as well as drastic changes of gradients of the nonlinear functions at certain saturated nodes which become unsaturated.

Using the given physical parameter values and a moderately fine mesh consisting of 252 nodes and 225 elements (216 rectangles and nine triangles), the problem was solved for 40 time steps. The time step values were computed using the following algorithm: $\Delta t_1 = d$, $\Delta t_k = 1.414$, $\Delta t_{k-1} \leq 600 d$, $k = 2, \dots, 40$. The seepage face boundary condition at the drain was treated in a simple manner using a trial-and-error procedure similar to that given by Neuman et al. (1974). For most of the time the Picard algorithm took four or five iterations per time step, whereas the Newton-Raphson algorithm took three iterations to converge within a head tolerance of 10^{-4} m. Both nonlinear algorithms produced pressure head solutions which were very close to each other. To show the effects of drainage and pumping on the flow system, the hydraulic head profiles along $y = 18.5$ m and $y = 29$ m are plotted in Figures 4.13 and 4.14, respectively. Note that there is quite a significant difference between head values at the two elevations. This indicates significant vertical flow, particularly in the vicinity of the tile drain. Also evident is the influence of pumping at the basement. This causes the reversal of the hydraulic gradient in the horizontal plane, $y = 18.5$ m, and from the tile drain toward the basement.

Finally, a plot showing temporal variation of the drain flux is presented in Figure 4.15. Once again, it is apparent that the Picard and the Newton-Raphson algorithms produced virtually identical results. The drain flux curve approaches the steady state value asymptotically, which implies a long-time attainment of equilibrium between the withdrawal and the replenishment of water in the flow system.

Table 4.4. Material Properties for the Landfill Problem.

Material type	K, m/d	ϕ	S_s , m^{-1}
Loam	5×10^{-2}	0.45	10^{-3}
Desiccated clay	5×10^{-3}	0.60	2×10^{-3}
Clay and till	5×10^{-4}	0.60	2×10^{-3}

Material Type	S_{wt}	n	α , m^{-1}	β	γ
Loam	0.05	2	0.5	2	1.
Desiccated clay	0.20	2	0.282	1.5	1.
Clay and till	0.20	2	0.282	1.5	1.

Constitutive relations:

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

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

$$\text{where } S_e = (S_w - S_{wt})/(1 - S_{wt}).$$

Figure 4.13. Hydraulic head distributions along $y = 18.5\text{m}$.

Figure 4.14. Hydraulic head distributions along $y = 29$ m.

Figure 4.15. Temporal variation of drain flux.

4.2.5 Transient Two-Dimensional 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 4.16. The purpose is to demonstrate another application of VAM2D 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 of 256 nodes (16 rows and 16 columns of nodes). Both flow and transport problems were solved. In this section, only the flow simulation result is presented. VAM2D input and output files for this flow simulation are presented in Section 10.2. The transport simulation will be dealt with in Section 4.3.5. The material properties used in the flow simulation are summarized in Table 4.5. 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 4.17 and 4.18 are pressure head and water saturation profiles, respectively. The ability of the VAM2D code to accommodate rapid response and contrasting properties of the soil system may be noted.

4.2.6 Steady-State Two-Dimensional Flow Beneath a Landfill

This problem 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 4.19 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 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 4.20 are simulation results. For the vertical section directly below the center of land disposal unit, water saturation profiles computed by VAM2D and a one-dimensional finite element code (VADOFT, Huyakorn et al., 1987) are compared in Figure 4.20a. There is reasonable agreement between the two-dimensional (VAM2D) and

Figure 4.16. Schematic description of the root zone problem, showing geometry of the problem (a) and the applied infiltration rate as a function of time (b).

Table 4.5. Material properties used in the simulation of root zone problem.

Layer no.	K, cm/d	ϕ	S_s cm ⁻¹	
1	350	0.41	0	
2	25	0.43	0	
3	10.8	0.45	0	

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:

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

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

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

Figure 4.17. Simulated profiles of pressure head in the root zone.

Figure 4.18. Simulated profiles of water-phase saturation in the root zone.

Figure 4.19. Schematic description of the simulated case of water flow and leachate migration in an unconfined system beneath a landfill.

Figure 4.20. Simulated saturation profiles and velocity field.

the one-dimensional (VADOFT) numerical solutions. It can be seen in Figure 4.20b, 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 4.20a.

4.2.7 Transient Infiltration Under Dry Soil Condition

This problem concerns transient vertical infiltration under an initially dry soil condition and a severely nonlinear soil moisture characteristics. The scenario considered is typical situation of infiltration in the vadose zone of a deep groundwater system in a semi-arid region. Shown in Figure 4.21 are the temporal variation of infiltration and characteristic curves used in the simulation. The functional description of these curves and other relevant hydraulic properties for the simulated case are presented in Table 4.6. The moisture characteristic curves plotted in Figure 4.21 are fitted curves derived from moisture data reported by Abeele et al. (1981) for solid Bandelier tuff. The water table was assumed to be located at a depth of 350 m below the soil surface. A column grid consisting of 101 rectangular elements and 202 nodes was adopted. The simulation was performed over a time period of 5 yr using target step values of 0.1 yr. To handle the highly nonlinear condition, the Newton-Raphson scheme with upstream weighting and lumping of storage matrix was used. The code took between 3 and 10 iterations per timestep to achieve satisfactory convergence. Shown in Figure 4.22 are simulated profiles of water saturation corresponding to 5 annual time values. As expected, the profiles exhibit steep fronts and varying shape in response to the temporal variation of infiltration.

4.3 SOLUTE 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 case involving advective-dispersive transport in an unsaturated porous medium. The problem concerns one-dimensional transport of a non-conservative species in an unsaturated soil slab identical to that described in Section 4.2.1. Velocities obtained by solving the corresponding unsaturated flow problem were used as input data for the current transport problem. Initial and boundary conditions required by the model are depicted in Figure 4.23 together with values of the physical parameters used.

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 $\Delta t = 0.01$ days. Typical velocity profiles used in the transport calculation are illustrated in Figure 4.24. It is important to recognize that for the unsaturated flow case considered, the

Figure 4.21. Infiltration data and moisture characteristic curves used in the simulation of the vadose-zone infiltration problem.

Table 4.6. Material properties used in the simulation of transient vadose-zone infiltration problem.

Saturated hydraulic conductivity, K	35 m/d
Saturated water content, ϕ	0.4
Specific storage, S_s	0 m ⁻¹

Constitutive relations:

$$k_{rw} = S_e^{3.69}$$

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

where

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

$$\alpha = 0.423 \text{ m}^{-1}, \beta = 2.22$$

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

$$S_{wr} = 0.025$$

Figure 4.22. Simulated profiles of water-phase saturation at 5 annual time values.

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

Discretization Data: $\Delta x = 1 \text{ cm}$, $\Delta t = .01 \text{ d}$

Figure 4.23. Schematic description and data for the problem of transport in a soil slab.

Figure 4.24. Typical velocity profiles used in the one-dimensional transport analysis.

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 4.25. The result of the mass balance calculation is displayed by the plots shown in Figures 4.26 and 4.27. The behavior of the mass balance error versus time relationship should be observed. Note that the mass balance error for this particular case is very small.

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. As illustrated in Figure 4.28, 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 4.7. 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 grid was a uniform 11×16 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: $\Delta t_1 = 0.01$ days, $\Delta t_k = 1.2\Delta t_{k-1} \leq 0.05$ 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 4.29 and 4.30 with the corresponding Galerkin solution obtained using the FEMWASTE code. Evidently, the overall agreement between the two numerical solutions is reasonable. The horizontal concentration distributions depicted in Figure 4.29 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.

We believe that the numerical oscillation problem experienced by FEMWASTE is associated with the manner in which the Galerkin approximation of the transport equation is performed. As described by Duguid and Reeves (1976) and Yeh and Ward (1981), the finite

Figure 4.25. Simulated concentration profiles for the one-dimensional transport problem.

Figure 4.26. Mass storage and mass decay curves computed by VAM2D.

Figure 4.27. Mass balance error versus time relationship for the 1-D solute transport problem.

Figure 4.28. Schematic description and data for the problem of two-dimensional transport in a soil slab.

Table 4.7. 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_o	-90 cm
Initial concentration, c_o	0
Longitudinal dispersivity, α_L	1 cm
Transverse dispersivity, α_T	0 cm
Apparent molecular diffusion, D^o	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 4.2.1.

Figure 4.29. Computed horizontal profiles for typical time values.

Figure 4.30. Computed vertical profiles for typical time values.

element formulation employed in FEMWASTE is achieved by applying Green's theorem to both the dispersive and the advective terms of the primitive transport equation. Such a formulation provides a convenient way to accommodate third-type material flux boundary conditions. Unfortunately, it is highly sensitive to errors in the computation of Darcy velocity and fluid flux values (see Huyakorn and Pinder, 1983, p. 199). In other words, small errors in the estimate of the fluxes can trigger sizable oscillations of concentration values adjacent to the flow boundary. Experience indicates that these oscillations may be dampened as time goes on or they may persist throughout the remaining simulation time period.

Unlike the finite element formulation used in FEMWASTE, the present formulation is achieved by using the transformed version of the transport equation and applying Green's theorem only to the dispersive term. This leads to the numerical scheme that is much less oscillation prone. In addition, the mass balance computational algorithm also works well in two dimensions. This is evident in the result presented in Figure 4.31. In Figure 4.31a, the behavior of the mass storage and decay curves may be noted. In Figure 4.31b, it is seen that the mass balance error for the problem solved behaves in a similar manner to that in the previous one-dimensional example problem. Of particular interest is the fact that the mass balance error corresponding to the medium grid with 176 nodes is substantially less than that corresponding to a coarser grid consisting of 96 nodes. The reason for this is the manner in which the finite element solution and the mass balance schemes are formulated. It may be recalled that the mass balance criterion used is an integral representation of the original transport equation. On the other hand, the numerical solution is formulated using the converted transport equation, which is equivalent to the original transport equation, provided the continuity equation for water flow is satisfied. If the velocity field and the water saturation distribution used in the transport analysis do not satisfy the continuity equation for flow, a significant mass balance error will be detected when the computed concentration is substituted into the solute mass balance integral equation. As depicted in Figure 4.31, the mass balance error is greater with the coarse grid than with the medium grid because the velocity field and water saturation distribution computed using the coarse grid are less accurate than those computed using the medium grid.

4.3.3 One-Dimensional Transport of a Three-Member Chain of Radionuclides

This problem is depicted schematically in Figure 4.32. The problem was selected to test the implementation of the upstream weighting and Galerkin schemes, and the programming features in VAM2D designed to handle chain decay and time dependent flux boundary conditions. VAM2D input and output files for this problem are presented in Section 10.5. The problem concerns transport of a chain of three radionuclides released from a source located at $x = 0$ in a confined porous medium reservoir. For the case of a straight three-member chain, an analytical solution can be found in Coats and Smith (1964). The flow region and the reservoir properties used in the present simulation are also depicted in Figure 4.33. The properties of the three radionuclide components employed are given in

Figure 4.31. Mass storage and decay curves and mass balance error computed by VAM2D.

Figure 4.32. Schematic description and data for the problem of one-dimensional multi-component transport.

Figure 4.33. Simulated concentration profiles for the case of straight chain, showing comparison of analytical and finite element solutions.

Table 4.8. Two cases involving straight and branch chains were simulated. For the branch chain, it was assumed that the mass fractions for transformation of component 1 to 3 and 1 to 2 are equal to 1/2. A decaying source with step release boundary condition was assumed at the inlet. For comparison purposes, the transport parameter values were selected to correspond to the data used in a previous study on a three-member straight chain transport simulation reported by Reeves and Cranwell (1981). This study utilized a block-centered finite difference technique that is of a lower order of accuracy than the consistent mass finite element approximation.

To obtain the finite element solution, the flow region was discretized into 20 linear line elements of equal length, thus giving $\Delta x = 32.8$ ft (~ 10 m) and a mesh Peclet number $Pe = 3.86$. (The mesh Peclet number is defined as $Pe = V\Delta x/D_L = \Delta x/\alpha_L$.) In view of the fact that the Peclet number well exceeds a critical value of 2, a numerical experiment was first performed to study the behavior of Galerkin and upstream weighted solutions. At first the problem was solved for 15 time steps using the Galerkin and the upstream weighted schemes with upstream weighting factor $\alpha = 0.1$. A constant time step value of 18.2 yrs was also used. For $t = 273.9$ yrs, the complete results (concentration distributions of all three components) obtained using the upstream weighted scheme are shown in Figure 4.33 and 4.34 for cases 1 and 2 respectively. Excellent agreement with the analytical solutions may be observed.

4.3.4 Two-Dimensional Transport in Uniform Groundwater Flow

This problem concerns two-dimensional dispersion of solute species released from a point source in the horizontal plane of uniform groundwater flow. It was selected to test the transport numerical schemes in the VAM2D in two-dimensions for single-component and multi-component simulations. Parameter values used to run the code are listed in Table 4.9. 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 $-360 \leq x \leq 1980$ and $0 \leq y \leq 300$ m. It represented the upper half of the modeled flow region because of symmetry about the x-axis. Three cases, two single-species and one chain decay transport of components 1 and 2, 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. Results obtained for the first two single-specie cases are depicted in Figures 4.35 and 4.36, respectively. For both of these cases, it was assumed that the contaminant source was non-decaying and contaminant leaching occurred at a uniform rate of $Qc_o = 704$ g/d per unit aquifer thickness. The numerical solutions from VAM2D 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 4.36, the numerical result obtained using a fine mesh with $\Delta x = 60$ and $\Delta y = 15$ m is also presented to provide an illustration of the convergence behavior of the numerical solution. Case 2 corresponds to a

Table 4.8. Parameter values for the problem of one-dimensional transport of three-member radioactive decay chains.

Component ℓ	<u>Radionuclide properties</u>			
	$t_{1/2,\ell}$ yrs	λ_ℓ yrs ⁻¹	R_ℓ	c_ℓ^0
1	433	0.0016	9352	1
2	15	0.0462	9352	0
3	6540	0.0001	9352	0

Case 1: straight chain	1 ----> 2 ----> 3
Case 2: branch chain	<div> </div>
($\xi_{31} = \xi_{21} = 0.5$)

Figure 4.34. Simulated concentration profiles for the case of branch chain, showing comparison of analytical and finite element solutions.

Table 4.9. 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_o (per unit thickness of aquifer)	704 g/(m.d)
Bulk density, ρ_B	1.46 g/cm ³
<u>Solute Component 1:</u>	
Decay coefficient, λ	$1.9 \times 10^{-4} \text{ d}^{-1}$
Distribution coefficient, k_d	0.308 cm ³ /g
<u>Solute Component 2:</u>	
Decay coefficient, λ	0
Distribution coefficient, k_d	0

Figure 4.35. Simulated profiles of dimensionless concentration along the x-axis (single-specie transport, case 1).

Figure 4.36. Simulated profiles of dimensionless concentration along the x-axis (single-specie transport, case 2).

field situation involving transport of hexavalent chromium. Observed plume data reported by Perlmutter and Lieber (1970) is compared with the VAM2D simulation result as shown in Figure 4.37. 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.

To demonstrate a further potential field application of the VAM2D code in the investigation of multi-component contaminant transport, a third case was also considered. In this case, it was assumed that component 1 decays to component 2, which has zero decay and distribution coefficients (conservative species). The source was treated as a decaying source and the initial mass fluxes of components 1 and 2 were 704 g/m.d) and 0, respectively. Simulated concentration profiles along the plume center line are depicted in Figure 4.38. The VAM2D results are compared against those obtained using the Laplace-Transformed Galerkin (LTG) solution scheme of Sudicky (1989). The agreement is excellent. The profiles behave in the manner expected because of contrasting transport properties of the two solute components.

4.3.5 Transient Transport in a Root Zone

This problem is associated with the flow problem described in Section 4.2.5 and Figure 4.16. Transport of pesticide uniformly applied over the top soil is considered. A first-type boundary condition of unit concentration was assumed at the top surface, and a second type (outflow) boundary condition was assumed at the bottom of the root zone. The transport simulation was performed for 20 time steps using the velocity and water saturation data obtained from the previous flow simulation. VAM2D input and output files for this transport problem are presented in Section 10.3. The corresponding files for the simultaneous flow and transport simulation are given in Section 10.4. Shown in Figure 4.39 is the plot of concentration profiles for five time values. The profiles behave in the manner expected for a layered system.

4.3.6 Leachate Migration from a Landfill

This transport problem is associated with the variably saturated flow problem described in Section 4.2.6. It was selected to demonstrate another potential application of VAM2D in the investigation groundwater contamination due to land disposal of toxic waste. Shown in Figure 4.40a and 4.40b are the transport scenario modeled and a steady-state contaminant plume predicted by VAM2D 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 in the saturated zone due to the effect of downward vertical groundwater flow components caused by a slight mounding of the water table.

Figure 4.37. Simulated and observed plumes of hexavalent chromium.

Figure 4.38. Simulated profiles of concentration along the x-axis (two-member chain transport, case 3).

(a)

(b)

Figure 4.39. Plot of concentration profiles for the root-zone flow and transport problems.

4.3.7 Simulation of Solute Transport in a Caisson Experiment

In this example, VAM2D was used to simulate an intermediate field-scale experiment conducted at Los Alamos in a large Caisson (3 m internal diameter by 6 m height). Data from this experiment have been reported by Nyhan et al. (1986). The experiment set up is shown schematically in Figure 4.41. The Caisson was filled with crushed Bandelier Tuff, which consists mostly of silicic glass and has a grain-size distribution similar to that of a silty sand. At the bottom of the Caisson, a drain was installed, covered with a coarse screen. Approximately 0.25 m of gravel was placed over the screen, and above this was placed approximately 0.25 m of coarse sand. Solute application was made uniformly at the top of the Caisson. Concentration breakthrough data were measured at six different depths by analyzing water samples collected from access ports using hollow fiber suction cups.

One-dimensional simulations of transport of bromide were performed using VAM2D and a column grid consisting of 55 elements. A summary of parameter values is presented in Table 4.10. These parameter values were based on the result of previous model calibrations by Huyakorn et al. (1987) and van Genuchten et al. (1987). The two cases referred to in Table 4.10 represent two estimates of the key transport parameters controlling the position and shape of breakthrough curves at various depths. Evidently, the measured concentration data indicate some deviations from the one-dimensional flow and transport assumptions due to possible influence of material heterogeneity and boundary effects. Case 1 may correspond to a faster velocity zone that occurred in part of the Caisson that intersected the 264-cm depth sampler. Case 2 parameter values were chosen to provide the best overall fit of breakthrough curves at depths over 264 cm. Comparisons of simulated breakthrough curves and measured data are depicted in Figures 4.42 and 4.43 for the two cases, respectively. It can be seen that agreement between the predicted and observed concentrations is reasonable.

Figure 4.41. Schematic description of Caisson experiment on solute transport in unsaturated crushed Bandelier Tuff.

Table 4.10. Parameter values for one-dimensional transport of bromide in the Caisson.

Effective porosity, ϕ	= 0.331
Water saturation, S_w	= 0.834
Soil bulk density, ρ_B	= 1.60 g/cm ³
Injection Br concentration, c^*	= 70 mg/l
Background Br concentration, c_o	= 0.0
 <u>Case 1</u>	
Darcy velocity, V	= 3.22 cm/d
Longitudinal dispersivity, α_L	= 0.50 cm
Pulse duration, T	= 5.43 d
 <u>Case 2</u>	
Darcy velocity, V	= 4.07 cm/d
Longitudinal dispersivity, α_L	= 2.5 cm
Pulse duration, T	= 6.0 d

Figure 4.42. Simulated and observed bromide concentrations (case 1 simulation).

Figure 4.43. Simulated and observed bromide concentrations (case 2 simulation).

PART II

USER'S MANUAL

Figure 5.1. Basic geologic environment for a low-level waste container (Frind et al., 1977; reproduced with permission of the authors).

(a)

(b)

Figure 5.2. Groundwater seepage due to mine dewatering or underground drainage operations.

Figure 5.3. Groundwater contamination caused by a landfill.

Figure 5.4. Soil and groundwater contamination caused by application of pesticides.

permeability versus water phase saturation and pressure head versus water phase saturation. These relationships may be supplied to the code using functional parameters.

Data required for the analysis of solute transport problems include 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, fluxes, and decay constants), groundwater velocities, water saturation, and initial and boundary conditions associated with the transport equations.

5.3 SIMULATION PROCEDURE

The general procedure for using VAM2D to simulate water 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).
- If a curvilinear grid is used, the x-y coordinates of all nodal points will need to be input. This grid may be automatically generated using conformal mapping procedures, or may be prepared visually, with digitizing equipment for easy input.
- 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.

Figure 5.5. Typical rectangular meshes generated automatically by the VAM2D code using the option of IXYRED = 0.

- 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

If a rectangular mesh is used by VAM2D, the mesh is automatically generated by the code when the required mesh parameters are specified. Note that the x- and y-coordinates correspond to the horizontal and vertical axis, respectively, if a cartesian coordinate system is used. If an axisymmetric coordinate system is used, x and y correspond to the radial and vertical axis, respectively. The finite element mesh parameters are specified as follows in the data input file:

Record type 12 (see Chapter 8)

NROWS:	Number of grid lines parallel to the x-axis.
NCOLS:	Number of grid lines parallel to the y-axis.
DXMAX:	Maximum value of spatial increment allowed in the x-direction.
DYMAX:	Maximum value of spatial increment allowed in the y-direction.
IXYRED:	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, = 3 if complete coordinate input is required, i.e., for a curvilinear grid.

For IXYRED=1, record types 13a and 13b data need to be supplied. For IXYRED=0, record type 14a data needs to be supplied. For IXYRED=2, record type 14b data needs to be supplied. For IXYRED=3 (i.e., a curvilinear grid), nodal x- and y- coordinates need to be supplied in group 13c. Note that when the control parameter for a curvilinear grid (group 5, col. 71-75) is set to ICURVL=2, the nodal coordinate data will be supplied from an external data file (TAPE 13), rather than in the main input file.

Record type 13a

Number of records = $\text{NCOLS}/8 + 0$ or 1.

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

Record type 13b

Number of records = $\text{NROWS}/8 + 0$ or 1.

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

Record type 13c

(1) x-coordinates of all nodes

Number of records = $\text{NP}/8 + 0$ or 1 (group 3, col. 41-45).

Col.	1-10	CORD(I,1):	x-coordinates of all nodal points in the sequential
	11-20	I = 1, NP	order.
	etc.		

(2) y-coordinates of all nodes

Number of records = $\text{NP}/8 + 0$ or 1 (group 3, col. 41-45).

Col.	1-10	CORD(I,2):	y-coordinates of all nodes in the sequential order.
	11-20	I = 1, NP	
	etc.		

Record type 14a

Col.	1-10	DX:	Starting value of spatial increment in the x-direction.
	11-20	DY:	Starting value of spatial increment in the y-direction.

21-30	XO:	Maximum value of x-coordinate.
31-40	YO:	Maximum value of y-coordinate.
41-50	SCFX:	Scale factor in the x-direction.
51-60	SCFY:	Scale factor in the y-direction.
61-70	XSTART:	Minimum value of x-coordinate.
71-80	YSTART:	Minimum value of y-coordinate.
	ISWAP:	Code for indicating the sequential number of the nodes in the rectangular mesh to be generated, = 0 if the nodes are sequentially numbered in the y-direction, = 1 if the nodes are sequentially numbered in the x-direction.

Record type 14b

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; = 0 if no.

Second subset

Each record contains the following information:

Col.	1-10	DELTA Y:	Spatial increment in the x-direction.
	11-15	ISTR:	Starting element column number.

16-20	IENDR:	Ending element column 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; and
 - (3) the sum of DELTAY* (IENDR-ISTR + 1) must be equal to YO-YSTART.

Note how the nodes are sequentially numbered along the shortest axis in Figure 5.4 to achieve a minimum matrix bandwidth. The parameter that specifies how the nodes are to be numbered is in record group 3, cols. 51-55.

Even when a rectangular mesh is used, 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 flow or transport analysis or a steady-state flow analysis, the initial distribution of the dependent variable to be solved must be supplied to the code. If the initial distribution is uniform, it is sufficient to supply constant default values of head and/or concentration to the code. The default initial head may be specified in terms of either pressure head (ψ_o) or hydraulic head (h_o). If the hydraulic head h_o is used, the user needs to tell the code to convert it to pressure head (unless the total head option is used) by setting input control parameter INTSPC = 1. In case of a variably saturated flow simulation, it is also possible to specify the initial condition in terms of the water contents (N.B.: not the saturations!) at the centroids of each element in the model domain. This option is selected by setting control parameter INTSPC=2. Note however, that this option can be used only if hysteresis is ignored (IHYST=0) and the entire domain is unsaturated. For a simulation involving hysteresis, both the initial pressure heads and initial saturations must be given.

In a case of a 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).

Boundary conditions can be given in terms of either the pressure head (or total heads) or concentration at boundary nodes, or in terms of the fluid or solute flux at boundary nodes. In case a dual flow and transport simulation is to be performed, boundary conditions for both the flow equation and the transport equation must be provided. In this case, the flow equation is considered equation no. 1 and the transport equation is equation no. 2. Therefore, boundary conditions pertaining to the flow equation are indicated by setting the dependent variable I.D. number to 1, and transport boundary conditions are indicated by setting the dependent variable I.D. number to 2 (see Chapter 8, input group 15). Conversely, when flow or transport are simulated separately, there is only one equation to be solved and the dependent variable I.D. number is always 1. Specification of a first-type boundary condition is very straight-forward and requires no further explanation. Specifying the nodal boundary condition values in the case of a flux-type boundary condition is more involved. The procedure is explained below by means of an example.

Suppose we wish to simulate migration of a contaminant through the unsaturated zone, where the contaminant originates from a leaky container placed on the soil surface. A close-up of the finite element grid just below the container is shown in Figure 5.6. The boundary nodes that are in contact with the container are represented with the solid circles and are arbitrarily labeled $i, j, \dots, m$. Other nodes are represented by open circles. Nodal spacings between the boundary nodes in the horizontal direction are $\Delta x_a, \Delta x_b, \dots, \Delta x_d$. Let's further assume that the container loses liquid at a rate of Q cubic meters per day. The liquid is distributed uniformly over the area (S, m^2) of the container which is in contact with the soil. The so-called *distributed liquid flux* is then $q = Q/S$ m/d. The contaminant concentration in the liquid is c_o gr/ m^3 . The *distributed solute flux* is thus $q \cdot c_o$ gr/(m^2/d).

We must now translate this distributed flux into the correct flux boundary conditions at the boundary nodes. Starting at node i , the procedure is as follows: The total liquid flux applied over the boundary segment between nodes i and j is $q \cdot \Delta x_a$. One-half of this is apportioned to node i and one-half to node j . In addition, node j receives one-half of the flux entering through the segment between nodes j and k . The resulting nodal flux values are called *integrated* (or concentrated) flux boundary conditions. For the current example, the integrated nodal fluid and solute flux boundary conditions are:

Figure 5.6. Example illustrating calculation of integrated nodal fluxes. Closed dots represent nodes along boundary segment receiving flux. Open dots represent remaining nodes.

<u>node</u>	<u>nodal fluid flux</u>	<u>nodal solute flux</u>
i	$\frac{1}{2}q\Delta x_a$	$\frac{1}{2}qc_o\Delta x_a$
j	$\frac{1}{2}q(\Delta x_a + \Delta x_b)$	$\frac{1}{2}qc_o(\Delta x_a + \Delta x_b)$
k	$\frac{1}{2}q(\Delta x_b + \Delta x_c)$	$\frac{1}{2}qc_o(\Delta x_b + \Delta x_c)$
l	$\frac{1}{2}q(\Delta x_c + \Delta x_d)$	$\frac{1}{2}qc_o(\Delta x_c + \Delta x_d)$
m	$\frac{1}{2}q\Delta x_d$	$\frac{1}{2}qc_o\Delta x_d$

In general, the integrated nodal fluxes are obtained by multiplying the areally distributed flux by the effective nodal length. The example also illustrates that the nodal fluid flux has dimensions of length x length/time = L^2/T .

Steady-state boundary conditions are handled simply by specifying the node numbers and prescribed concentration or solute mass flux and fluid flux values. Transient boundary conditions are also handled in a convenient manner by specifying the node numbers and relationships of time versus concentration or flux values. The code admits both continuous and stepped temporal variations (Figure 5.7). A continuous variation is represented using a 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.

Chained decay source boundary conditions can also be handled by VAM2D. In this case, the code needs data for the node numbers of the nodes representing the decaying sources. Data describing the source characteristics are also needed. These data include the leach time duration of the source, source decay coefficients, and initial solute mass flux or concentration data. The analytical solution of the Bateman equations is used to compute the source concentration and solute mass flux released from the source at a specified time value. This computation is performed for all components along each chain (or reaction path). The number of paths is 1 for a straight chain and greater than 1 for a branched chain.

5.6 GENERAL GUIDANCE ON SELECTION OF GRID SPACINGS AND TIME STEPS, AND THE USE OF SOLUTION ALGORITHMS

5.6.1 Grid Spacing

In designing a finite element grid, one should select nodal spacings that will yield reasonable approximations to the expected moisture profiles, head and/or concentration distributions. Small nodal spacings should be used in the zones where head (and/or

(a)

(b)

Figure 5.7. Modeled approximations for continuous and discontinuous variations of prescribed function at node I.

concentration) gradients or moisture fronts are steep. The nodal spacings may be gradually increased in the zones where no abrupt changes in hydraulic conductivities occur and the gradients are fairly mild. If a curvilinear grid is used, the total head formulation should be used for flow simulations.

For solute transport modeling problems, the Peclet number criterion can be used to determine an appropriate mesh spacing. The local grid Peclet number is defined as

$$P_e = \frac{\Delta x}{\alpha}$$

where Δx is the element dimension and α is the dispersivity. The general rule is that the local Peclet number should not exceed a value of 4. In case where flow is steady state, the Peclet number should not exceed 2 or 3. When the grid Peclet number exceeds the indicated values, oscillations in the computed concentrations may occur, i.e., negative concentration values and relative concentrations greater than 1. The use of Crank-Nicholson time weighting scheme is more susceptible to oscillations than the use of a fully implicit time approximation. It is not always practical, for instance when dispersivities are very small, to refine the grid far enough that the Peclet number criterion is satisfied. As an alternative, one may use a relatively coarse grid, combined with upstream weighting of the transport solution. Upstream weighting is quite effective for reducing numerical oscillations, however, at the expense of increasing numerical dispersion.

5.6.2 Time Stepping and Iteration Schemes

VAM2D offers two different approaches for the selection of time steps in transient simulations. These are controlled by the input parameter ITSGN (see Chapter 8, Group 3). The user can either select the time step values to be used during the simulation in advance (ITSGN=0,1,2), or instruct VAM2D to determine the optimal time step size during the simulation itself (ITSGN=3). The latter option is useful for variably saturated flow simulations involving highly nonlinear conditions and/or time-varying boundary conditions.

Using the first approach, the user specifies the number of time steps (NTS) to be taken during the simulation. The time step values themselves are either provided directly in the input data file, or VAM2D constructs an internal table of time values, as specified in the data input file. The NTS time values represent target time values. For a transport simulation, the target time steps are also the actual, computational time steps used by the code. For a variably saturated flow simulation on the other hand, each target time step may be divided up into 2 or more computational time steps. At the start of each new target time step, the computational time step is set equal to the new target time step. Each time the solution fails to converge within a prescribed maximum allowable number of iterations

(NITMAX), the computational time step is reduced by a factor of 1/2 of its current value. The iteration process continues until either convergence is achieved or the maximum allowable successive reductions of time step (IRESOL) is exceeded. If convergence occurs, the code continues the analysis (over the remaining portion of the target time step) using the most recent value of computational time step. This time step control marching procedure is used over the entire flow simulation period. If convergence does not occur and IRESOL is exceeded, VAM2D execution is automatically terminated. One consequence of this scheme is that if a combined flow and transport simulation is performed, the transport analysis is performed using the target time steps, while the flow analysis may use smaller computational time steps to ensure convergence.

In VAM2D, a transient transport analysis can be performed concurrently with the associated transient flow analysis. If this option is used, the code will assume that the mesh and the target time values for the flow problem also apply to the transport problem. Another option available is to perform the transport simulation separately from the flow simulation. Using this option, the finite element mesh for flow and transport is still the same but time steps for both analyses may be different. The user can specify to the code time values where velocity and water saturation output is to be written on a backup file on unit 9. These target time values (which need not correspond to the target time values for the non-linear flow analysis) can then be adopted for the subsequent transport analysis. The selection of time steps for the transport simulation can be made based on the use of the following Courant's criterion:

$$\Delta t \leq \Delta x / (V_{\text{solute}})$$

where V_{solute} is a characteristic solute velocity defined as $V_{\text{solute}} = v/(\theta R)$, in which v is the Darcy velocity, θ is the water content, and R is the retardation coefficient.

There is no strict guide that can be given for the selection of appropriate time step values for a transient variably saturated flow analysis. For this reason, VAM2D has the option to adjust the time step size automatically during a transient flow simulation. This option is selected by setting the control parameter ITSGN equal to 3. In this case, parameter NTS represents a maximum allowable number of time steps. The procedure used by VAM2D for adjusting the optimal time step in a transient flow simulation is as follows: Before starting a new time step in a transient flow simulation, the code adjusts the time step size depending on the number of iterations that was required to reach convergence at the just completed time step. If the solution converged rapidly, the time step size is increased. If, on the other hand, the number of iterations approached NITMAX, this is taken as a sign that the time steps size was too large and its value is reduced before starting the new time step. If the flow solution failed to converge at all in NITMAX iterations, VAM2D uses the same procedure as outlined above: The time step size is reduced by half and the solution is attempted again. If no convergence is obtained after IRESOL successive reductions of the time step size, VAM2D execution is terminated.

The variably saturated flow simulation can be performed using either the Picard or the Newton-Raphson solution algorithm. We generally recommend the use of the Picard algorithm with mass lumping option for cases where convergence difficulties are not expected. For certain steady cases involving highly nonlinear soil moisture characteristics, the use of the Newton-Raphson algorithm with mass lumping and upstream weighting is preferable, particularly when its counterpart fails to converge within a reasonable number of iterations (say between 10 and 20). The Newton-Raphson procedure is more strongly convergent than the Picard method, but requires substantially more operations per iteration. In order to achieve optimal computational efficiency for transient flow problems, VAM2D allows the user to specify the use of Newton-Raphson for certain time periods during a simulation and the use of Picard iteration during remaining time periods. For instance, the user can select the Newton-Raphson method for periods of infiltration, where convergence problems are most likely, and use of Picard iteration for periods of redistribution. Optionally, the VAM2D code will automatically switch from Picard to Newton-Raphson when convergence difficulties are encountered. If this option is enabled (by setting ITSGN=3 and ISELSC=1), the code will switch to Newton-Raphson iteration if the code fails to converge in a specified number (NITMAX) of iterations, and back to Picard if rapid convergence is obtained.

5.7 MASS BALANCE ASSESSMENT

At the conclusion of a steady-state analysis or at the conclusion of each (target) time step of a transient analysis, the VAM2D code can perform an assessment of mass balance. As part of a problem setup, the user has the option of specifying whether volumetric flow (or solute mass) balance and/or flux calculations are to be performed. If either are to be done, the user must specify the boundary nodes where integrated flux values are to be calculated. The sign convention adopted for summing these fluxes is positive for influent and negative for effluent fluxes.

For the flow simulation, the volumetric balance summary printed to file number 6 includes the following:

1. Total flow rate due to boundary flux and sinks,
2. Rate of fluid accumulation,
3. Volumetric flow balance error,
4. Normalized flow balance error, and
5. Cumulative volumetric storage of fluid.

The first item is a summation of influent and effluent fluid fluxes calculated at the user-specified nodes. For example, if a steady-state flow field is simulated and all boundary and source/sink nodes are identified for the flow balance, then the total flow rate should be identically zero. The second item is the fluid accumulation rate. This quantity is an element-by-element summation of the change in fluid volume from one time step to another. Note that fluid accumulation rate is identically zero for steady-state flow fields. Volumetric flow balance error, the third item, is the difference between the previous two items. The fourth item is a normalized version of the flow balance error. It uses a summation of the absolute value of boundary and source/sink integrated nodal fluxes as the normalizing quantity. Obviously, the user-specified nodes for the flow balance or flux calculations influence the flow balance characterization of a simulation. These nodes must be selected to represent all fluxes in and out of the problem if the resultant calculations of fluxes are to accurately reflect the mass balance of the problem. The final item is the current value of cumulative volumetric storage of fluid inside the flow domain.

For the transport simulation, the solute-component mass balance summary printed to file unit number 6 includes the following:

1. Total net value of dispersive and advective solute mass fluxes,
2. Net rate of solute mass decay and transformation,
3. Net rate of solute mass accumulation (storage + decay + transformation),
4. Mass balance error,
5. Normalized mass error,
6. Cumulative mass cumulation, and
7. Cumulative mass decay and transformation.

The first item is the net sum of integrated values of dispersive and advective fluxes at the user-specified nodes. The second item is the sum of mass decay rate of the component being considered and the rate of mass transformation to that component. The third item is the net sum of the rate of mass storage and the second item. The fourth item is the mass balance error computed by taking the difference between items 1 and 3. The fifth item is a normalized mass balance error obtained by normalizing item 4 with respect to absolute sums of all fluxes and mass storage, decay and transformation terms. The last two items, 6 and 7, are cumulative values of net mass accumulation, and decay and transformation, respectively.

5.8 DATA PREPROCESSING AND OUTPUT POSTPROCESSING

An interactive data preprocessor code that facilitates the preparation and editing of a proper formatted input file for running VAM2D has recently been developed. This processor is written in C for convenient use on a personal computer using MS DOS operating system. Output from the preprocessor is written on a file that can be used directly as an input file on unit 5 for VAM2D. As an alternative option to using the preprocessor, the user may elect to prepare manually the required input data file for VAM2D. In this case, the input data preparation guide given in Chapter 8 needs to be used.

For graphical analysis of VAM2D output results, use of the auxiliary output files (FORTRAN Unit 10 and Unit 11) is recommended. These files contain nodal and elemental values of the various quantities of interest, e.g. pressure heads, saturations, concentrations, in a general x-y-z format which is readily accepted by a variety of data analysis software, including spreadsheets and contouring packages.

6 CODE STRUCTURE

6.1 SUBROUTINE LIST

The VAM2D code contains a main program and 35 subroutines. The functions of these program segments are as follows:

<u>PROGRAM SEGMENT</u>	<u>FUNCTION</u>
MAIN Program	Reads and writes input data and calls a number of key subroutines.
ASSEMV	Assembles element matrices.
BALCHK	Computes nodal values of fluxes and water and solute mass balance for the entire solution region.
BATEMN	Computes the Bateman analytical solution for a decaying source.
BUPDAT	Updates source boundary conditions.
DEFINT	Initialize nodal hysteresis parameters.
DSWCRU	Computes upstream weighted values of nonlinear soil functions at element centroids.
DSWCOM	Compute values of nonlinear soil functions at element centroids.
DSWFUN	Computes moisture capacity function.
DXYGEN	Generates spacings (Δx and Δy) of vertical and horizontal grid lines of the rectangular grid.
EBFIND	Computes maximum bandwidth of the global matrix.
EBFOR1	Computes seepage element matrices for rectangular elements.

PROGRAM SEGMENT**FUNCTION**

EBFOR2	Computes transport element matrices for rectangular elements.
EIBCHK	Updates boundary conditions for the nodes having infiltration or evaporation.
EVISET	Identifies the global sequential numbers of the nodes having infiltration or evaporation, and computes nodal areas and initial estimates of flux values.
FIXQ	Computes the integrated flux values for the seepage nodes and determines the total flow rate from the seepage faces.
FIXQEV	Updates nodal flux values for the nodes having infiltration or evaporation.
HDEST	Obtains the first estimate of head values at the current time level.
HFINTP	Determines the prescribed head or flux values by interpolation.
HSFIXB	Identifies the seepage face nodes and initializes boundary conditions at these nodes to a zero pressure head value.
MESHGN	Generates nodal coordinates and element connections for a simple rectangular grid.
PBC	Allocate prescribed Dirichlet and flux boundary conditions.
PKWFUN	Computes relative permeability function.
RFINTP	Performs linear interpolation using tabulated values of root effectiveness function versus elevation (depth coordinate).
SFCHCK	Updates the boundary conditions on the seepage faces.

<u>PROGRAM SEGMENT</u>	<u>FUNCTION</u>
SOLVEC	Solves a linear set of algebraic equations using a Gauss elimination scheme for an unsymmetric banded matrix.
SOLVEP	Solves a set of algebraic equations taking into account the symmetric banded feature of the coefficient matrix.
SWHFUN	Computes water saturation function.
SWICOM	Computes nodal and element water saturation values using pressure head from previous time value.
SSUPDT	Updates values of effective storage coefficient at element centroids.
TLOOP1	Computes nodal values of the specified dependent variable (head or concentration) for the specified number of time steps.
TLOOP2	Computes nodal values of both head and concentration for the specified number of time steps.
TRANSP	Implements the procedure for constrained maximization of the water uptake by plant roots. This procedure is described in Section 3.2.5.
TRANST	Computes effective surface area of the nodal columns in the root zone, and computes values of root effectiveness function at the nodes in the columns.
UPDATE	Update nodal values of hysteresis parameters.
VARCAL	Performs updating of boundary conditions and setting nonlinear iteration loop.
VANISO	Computes unsaturated hydraulic conductivity for variable anisotropy case.

PROGRAM SEGMENT

FUNCTION

VSWCOM	Computes values of water saturation and Darcy velocity components at element centroids.
WYSET	Sets the magnitude and sign of the upstream weighting factors, α and β , associated with the upstream weighting functions.
ZPRCON	Writes output at user selected time value.

6.2 INTERNAL DATA STRUCTURE

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

(1) Material properties. These data are read in and stored in three common blocks labeled MDATA, RDATA, and VARANI, respectively. The block MDATA contains material numbers and values of hydraulic and transport properties of different porous materials. The block RDATA contains properties of solute species. Finally, the block VARANI contains values of the variably anisotropy parameters for each material type.

(2) Nodal coordinates and element nodal connections. These data are either read in or generated by the code. They are stored in the common blocks labeled as WAVE.

(3) Boundary condition data. These data are read in and stored in two common blocks labeled DBATA and FDATA. The block BDATA contains node numbers and prescribed values of the dependent variables to be determined, i.e., hydraulic head, pressure head or concentration. The block FDATA contains node numbers and values of nodal fluxes.

(4) Initial condition data and computed values of dependent variables with time level. These are also stored in the common block labeled WAVE.

(5) 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

ized below. These must be observed by the user when applying the code to practical problems.

Maximum total number of nodal points	= 5000
Maximum total number of elements	= 4852
Maximum number of time steps (unlimited when automatic timestep adjustment option is used)	= 500
Maximum number of different sets of material properties	= 20
Maximum number of steady-state Dirichlet boundary conditions	= 309
Maximum number of steady-state flux boundary conditions	= 1212
Maximum semibandwidth of global coefficient matrix for fluid flow modeling	= 99
Maximum full bandwidth of global coefficient matrix for transport modeling	= 99
Maximum number of time-dependent, Dirichlet boundary nodes	= 50
Maximum number of time-dependent, flux boundary nodes	= 50
Maximum number of nodes for which flux computation is required	= 309
Maximum number of elements subjected to evaporation or infiltration	= 101
Maximum number of nodes subjected to evaporation or infiltration	= 202
Maximum number of observation nodes	= 75

Maximum number of seepage faces	= 10
Maximum number of nodes in each seepage face	= 30
Maximum number of seepage face nodes	= 100
Maximum number of plant nodal columns	= 35
Maximum number of plant species	= 5
Maximum number of elements in the root zone	= 155
Maximum number of nodes in the root zone	= 350
Maximum number of solute species for chain decay transport modeling	= 4
Maximum number of nodes representing decaying sources	= 20

6.4 INITIALIZATION

All of the important variables are initialized in the main program. The initialization procedure is outlined in Table 6.1.

6.5 RESTART PROCEDURE

A restart option is provided in the code to continue the solution of time-dependent problems. To use this option, the user must provide data for the initial nodal values of the dependent variables. These nodal values are to be supplied as input data in data file number 5. If the restart option is selected, the user should adopt the following procedure:

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

(2) Prepare input data for the file number 5 of the restart run in the usual manner, keeping in mind that data type 19 "initial value cards," can be readily obtained from the contents of file number 8. Note also that the variable NONU of data type 3 must be set equal to 1 and the variable NPIN of data type 6 must be set equal to the total number of nodal points in the finite element mesh.

Table 6.1. Initialization of Important Variables.

ARRAY VARIABLE	INITIALIZATION PROCEDURE
IPROP	IPROP(1) through IPROP(NE) are initialized to the default value of 1. This means that initially the code assumes that the material number corresponding to each element is 1.
HINT	HINT(1,1) through HINT(NP,NDF), where NP = number of nodes and NDF = number of dependent variables, are initialized to the default values which are read in by the code.
VELX	VELX(1) through VELX(NE), where NE = number of elements, are initialized to the default value, VCX, which is read in by the code.
VELY	VELY(1) through VELY(NE) are initialized to the default value VCY, which is read in by the code.

7 DATA FILES

There are five data files in the code. These are described as follows.

1. File number 5. This is the card 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 and their formats are provided in Chapter 8, which deals with input data.

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, which deals with output.

3. File number 8. This is the output file containing nodal values of the dependent variables which correspond to 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. This file (TAPE 8) contains the following information:

- Title Heading giving final time value; written in the FORMAT (20A4).
- List of Nodal Values of the unknown function (head or concentration, depending on whether one is dealing with flow or transport) at the final time level. For a hysteretic flow simulation, the element values of water saturation and wetting-drying index are also written to the TAPE 8 file. These values are written in (8E10.3) format.

The nodal values in TAPE 8 can be used as an initial condition for the next flow or transport restart run (not flow to transport). To do this, the user should delete the heading record of the TAPE 8 file and append this file onto the TAPE 5 file (see section 8.2 for details on TAPE 5 input data set up). Note that the TAPE 8 file corresponds to card type 18b. Next, the user should edit the input TAPE 5 file to set the initial condition control parameters NONU (record group 3, col. 66-70) equal to 1, and NPIN (group 5, cols. 11-15) equal to the total number of nodal points in the mesh.

4. File number 9. This file contains saturation and Darcy velocity data in binary format. If a transport simulation is performed, the flow information is read from the TAPE 9 file. This file is written when the flow simulation is performed and the value of the output control parameter NVWRIT is greater than 0. For each user-selected time step of the flow simulation, this output file (Tape 9) contains the following information, written in binary format:

- Title heading, giving the time value.

- List of element values of the x and y components of Darcy velocity.
- List of element water saturation values.
- 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.

The output file TAPE 9 from the flow simulation can be used as a direct input into the subsequent transport simulation. To do this, the user should proceed by editing the main datafile as follows:

- Set the control parameter NVREAD (group 5, cols. 1-5) equal to 2. This directs the code to read velocity and saturation data from TAPE 9.
- Make sure that IMBAL (record group 5, col. 46-50) is set to the value used in the flow simulation. This is necessary to insure data compatibility and avoid I/O format error.

5. File number 10. This file is written when the value of the plotting control parameter NPLOT (record group 5, col. 31-35) is greater than zero, and/or output control parameter NPRCON (group 5, col 61-65) is greater or equal than one.

For NPLOT=n, the output file TAPE 10 contains the following data for each selected time step/time value:

- Heading, giving the time step value.
- Nodal x and y coordinates followed by the nodal values of the dependent variables pressure head and/or concentration, written in Format: 7(E10.3,1X).

6. File number 11. This file is written when a flow simulation is performed, IMODL = 1 or 2 (group 3, col. 1-5) and NVPR is greater than zero, and/or NPRCON is greater or equal than one. The file TAPE 11 contains the following data for each selected time step/time value:

- Heading, giving the time step value.
- x and y coordinates of the element centroids followed by values of element water saturation, water content, x and y components of the Darcy velocity, magnitude of the velocity and angle of the velocity vector, written in Format: 8(E10.3,1x).

Velocity vectors can be plotted this way using the SURFER™ plotting software, via the POST option of the TOPO module.

7. File number 13. This datafile is used to read in nodal x- and y-coordinates when the curvilinear grid control parameter (group 5, col. 71-75) is set to ICURVL=2. The data format for the unit 13 file is given in data input group 13c. Use of the ICURVL=2 option is recommended when dealing with large grid, since it allows the main data input file to remain much smaller.

8 INPUT DATA PREPARATION

8.1 GENERAL CONSIDERATIONS

VAM2D is designed to perform the analysis of one problem or several consecutive problems in a single computer run. Several features are incorporated into the code for automatic generation of a substantial portion of the input required for the finite element analysis of each problem. These are summarized as follows:

- (1) Automatic mesh generation. The mesh generation is limited to a rectangular grid consisting of linear rectangular elements. Each grid must have constant number of nodal rows and constant number of nodal columns. The grid spacings can be uniform or variable.
- (2) Default initial value option. This option is invoked by setting the input variables NONU and NPIN equal to zero. When this is the case, all nodal values of the dependent variables will be set equal to the default initial values.
- (3) Default velocity and default water saturation option. This option is invoked by setting NVREAD equal to zero.

8.2 RESTART PROCEDURES

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

- (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 (group 5, cols. 51-55) equal to 1.
- (2) Prepare input data for file unit 5 of the restart run in the usual manner but keeping in mind that Record Type 18 and 22 initial value can be derived from information contained in file unit 8. Note also that the variable NONU (group 3, cols. 66-70) must be set equal to 1 and NOWRIT must be set equal to 0.

8.3 INPUT RECORDS

The main stream of input data is to be supplied from input file unit 5. The VAM2D code simulates two-dimensional flow and solute transport in a variably saturated medium. The program can solve the following problems: (1) variably-saturated flow, (2) transport of single component or multi-component chain in a variably saturated porous medium, and (3) combined flow and transport. The main stream of input data is to be supplied from input file unit 5. To facilitate data entry, the input data is divided into groups, arranged as follows:

1. Number of problems to be solved
2. Problem title
3. Simulation control parameters
4. Time stepping and iteration control parameters
5. Input and output control parameters
6. Temporal discretization data
7. Default initial values
8. Element property numbers
9. Hydraulic parameters of soil
10. Soil physical transport parameters
11. Soil-solute transport parameters
12. Mesh parameter specification
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18. Initial nodal value data
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20. Element Darcy velocity data
21. Element water saturation data for transport simulation
22. Initial element water saturation data for hysteretic flow simulation
23. Boundary nodal data
24. Evaporation, infiltration and seepage face data
25. Plant species data
26. Root zone element and node data
27. Observation node data
28. Velocity file output time specification data

The above sequence must be strictly followed when entering data into the program. The selection of units to be used is arbitrary (e.g., hour or day for time, centimeter or meter for length) but must be consistent. Where appropriate the type of unit (e.g., L(ength), T(ime), M(ass), etc.) for the input variable is given together with the format description. Following are descriptions of the input variables and data formats.

1. Number of problems (I5)

One record.

Col. 1-5 NPROB: Number of problems to be solved in this run.

*** The following record types are to be repeated for each problem.

2. Problem title (A80)

One record.

Col. 1-80 TITLE: Title of problem.

3. Simulation control parameters (1615)

One record.

Col.	1-5	IMODL:	Parameter indicating the type of modeling required; = 0 for solute transport modeling, = 1 for water flow modeling, = 2 for simultaneous flow and transport modeling.
	6-10	IHYST:	Parameter indicating if hysteresis is to be included in flow simulation; = 1 if yes, = 0 if no. (Set IHYST = 0 if IMODL = 0.)
	11-15	IANI:	Parameter indicating if variable anisotropy of hydraulic conductivity is to be included in flow simulation; = 1 if yes, = 0 if no. (Set IANI = 0 if IMODL = 0.)
	16-20	INTSPC:	Parameter specifying if initial head values supplied to the code by the user are given in terms of pressure head or hydraulic head; = 1 if hydraulic head, = 0 if pressure head. = -1 if initial pressure head values supplied to the code are to be converted to initial hydraulic head values. Set INTSPC = 0 if dealing with the transport equation (IMODL = 0). (Note: A special option is available if the initial condition is given in terms of elemental water contents; use INTSPC=2 in this case.)
	21-25	ICHAIN:	Parameter indicating if chained decay reactions or decaying source conditions are to be accounted for in the transport simulation; = 1 if yes, = 0 if no.

When only flow simulation is required (IMODL = 1), ICHAIN is set to zero.

26-30	ISSTA:	Parameter indicating if a steady-state analysis of the problem is required; = 1 if yes, = 0 if no.
31-35	ITSGN:	Parameter indicating if simulation time values are to be generated by the code; = 0 if no, = 1 if yes and time values are to be computed using generated time steps, = 2 if yes and time values are to be computed using specified time step values. = 3 if yes and timesteps are to be computed during the simulation.
36-40	NTS:	Number of target time steps (see Section 5.6). Set = 1 if a steady-state analysis of the problem is required. If parameter ITSGN=3, NTS represents the maximum allowed number of timesteps.
41-45	NP:	Total number of nodal points in the finite element grid.
46-50	NE:	Total number of elements in the finite element grid.
51-55	ISWAP:	Parameter indicating the sequential numbering of the nodes in the rectangular mesh to be generated; = 1 if the nodes are sequentially numbered in the x-direction, = 0 if the nodes are sequentially numbered in the y-direction. The purpose of ISWAP is to achieve a smaller matrix bandwidth; nodes should be numbered sequentially in the direction that contains the fewest number of grid lines.
56-60	IAXSYM:	Parameter indicating if the problem is axisymmetric with x and y corresponding to radial and vertical coordinates respectively;

= 1 if yes,
= 0 if no.

61-65	NMAT:	Number of different porous materials.
66-70	NONU:	Parameter indicating if initial condition values are nonuniform; = 0 if no, = 1 if yes and initial condition data are to be input as part of this input file (see group 18 and 22), = 2 if yes and initial condition data are to be supplied by reading from a file on unit 8. <u>Do not use the NONU = 1 option if dealing with multispecies solute transport simulation.</u>
71-75	NEIEVP:	Number of finite elements that are subject to infiltration or evaporation.
76-80	NPLANT:	Number of different plant species.

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

One record.

Col.	1-5	IKALL:	Parameter indicating the type time stepping scheme required for transport equation; = 1 for backward difference scheme, = 0 for central difference scheme. Note IKALL is automatically set to 1 if steady-state analysis is required.
	6-10	INEWT:	Parameter indicating the type of iterative procedure to be used in solving the variably-saturated flow equation. = 0 for Picard procedure = 1 for Newton-Raphson procedure. INEWT is set to 0 when dealing with the transport model only (IMODL = 0).

11-15	NITMAX:	Maximum number of non-linear iterations allowed per time step. If only solute transport is required (IMODL = 0), NITMAX is set equal to 1. Otherwise set NITMAX equal to the desired maximum number of iterations per time step.
16-20	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). Set to zero or leave blank if transport simulation only is required (IMODL = 0).
21-25	ILUMP:	Parameter indicating if mass lumping procedure is to be applied in formulating the element matrix of the flow equation; = 1 if yes, = 0 if no.
26-35	HTOL:	Absolute iteration tolerance for head during flow simulation (L). For a transport simulation, HTOL is automatically set = 0.0.
36-45	RELCON:	Relative iteration tolerance for head during flow simulation. The combined convergence tolerance is: $TOL = HTOL + RELCON \times \hat{h}_i^{t+\Delta t}$ where $\hat{h}_i^{t+\Delta t}$ is the estimated nodal pressure head at the new time value.
46-50	IUPSTR:	Upstream weighting control parameter for relative permeability; = 1 if upstream weighting is required; = 0 otherwise.
51-55	INSTOC:	Parameter indicating the procedure to be used in computing the storage term of the Newton-Raphson formulation of the flow problem; = 0 if computed in terms of $(dS_w/d\psi) \partial\psi/\partial t$, = 1 if computed directly from $\partial S_w/\partial t$. Leave blank if not used.
56-60	ISELSC:	Parameter indicating if a combined use of Newton-Raphson and Picard nonlinear schemes is

to be made in the transient simulation of the flow problem;
 = 1 if yes,
 = 0 if no.

61-65 NSEEP: Number of seepage faces.

5. Input and output parameters

5-A. Control parameters (1615)

One record.

Col. 1-5	NVREAD: Parameter specifying if element velocity and water saturation data are to be input; = 0 if no velocity and saturation input are needed (this option is used for a flow run), = 1 if the velocity and saturation data are to be included in this data file (this option is used for a transport run when the flow is steady state), = 2 if these data are to be input using a separate data file unit number 9. Note: NVREAD is set to 0 if IMODL = 1 or 2.
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6-10	IOUTLT: Parameter indicating if boundary node data (see group 23) are to be read in for writing boundary fluxes (required for mass balance computation); = 1 if yes, = 0 if no.
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11-15	NPIN: Number of nodes for which initial nodal values are to be input as part of this input file. NPIN is automatically set = 0 unless NONU = 1. Set NPIN=0 if initial water content data are to be read in for a flow simulation (INTSPC=2).
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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,
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- = 3 if mesh and initial condition data printouts are not needed.
- 21-25 NVWRIT: Parameter specifying if computed values of element velocities and water saturation are to be written on file unit 9;
 = 0 if no,
 = 1 if yes and output is to be written for each time step;
 = 2 if yes and output is to be written for selected time steps as specified in record group 28.
 Note: NVWRIT is set to 0 if IMODL = 2.
- 26-30 NVPR: Parameter controlling printout of computed element velocities and water saturation;
 = 0 if no output is to be written,
 = n if the output is to be written for each nth time step.
 Note: Output times are under program control when NPRCON > 0 is used. In this case, set NVPR=0 if no velocity output is desired, otherwise set NVPR=1 to include velocity output.
- 31-35 NPLOT: Parameter indicating if time and computed nodal values of the variables concerned (head, saturation, or concentration) 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 nth time step.
 Note: The output times are under program control when NPRCON > 0 is used. In this case, set NPLOT=0 to suppress plot file output, or NPLOT=1 to write plot file output.
- 36-40 NSTEP: Parameter controlling printout of computed nodal values;
 = 0 if no output is to be written,
 = n if the output is to be written for each nth time step.
 Note: The output times are under program control when NPRCON > 0 is used. In this

case, set NSTEP=0 if no nodal output is desired,
or NSTEP=1 to write nodal values.

- 41-45 IOBSND: Parameter indicating if values at some specified nodes are to be recorded for all time steps (see group 27);
 = 1 if yes,
 = 0 if no.
 Note: IOBSND should be set to zero if ITSGN=3 is used.
- 46-50 IMBAL: Parameter specifying if mass balance calculation is required,
 = 1 if yes,
 = 0 if no.
- 51-55 NOWRIT: Parameter indicating if computed values of head or concentration at the final time level are to be written on file unit 8;
 = 1 if yes,
 = 0 if no.
- 56-60 IPRCHK: Print check option parameter;
 = 1 if element matrix and boundary condition print check is required,
 = 0 if no.
 Note: IPRCHK should be set to 0.
- 61-65 NPRCON: Output control parameter;
 = 0 if output is desired at fixed time step intervals (see NVPR, NPLOT, NSTEP),
 = n if output is desired at n selected time values.
- 66-70 ITOTHD: Parameter indicating if total hydraulic head formulation is to be used for flow solution;
 = 1 if yes,
 = 0 if no, solve in terms of pressure head.
 Note: ITOTHD is used only in combination with a curvilinear grid. Set ITOTHD = 1 for flow solution when a curvilinear grid is used.
- 71-75 ICURVL: Curvilinear grid option;
 = 1 if yes,
 = 0 if no, rectangular grid used,

= 2 if yes and nodal coordinate data (group 13c) is to be read from an external data file, rather than supplied in the primary input file.

76-80 IPTPRT: Head output option for flow solution
 = 0 Output of actual dependent variable (pressure head or total head),
 = 1 Convert total hydraulic head to pressure head when writing output files.
 Note: IPTPRT is only used when ITOTHD = 1, otherwise this parameter is ignored.

5-B. Output time values (8E10.3)

*** Omit if NPRCON = 0

Col.	1-10	TMPRC(I): Time values for which output is desired (T). I=1, NPRCON
	11-70	
	etc.	

6. Temporal discretization data

(a-1) Time discretization parameters (4E10.3)

*** Omit if ITSGN (see group 3, Col. 31-35) = 3

One record.

Col.	1-10	TIMA: Initial time value (T).
	11-20	TIN: Initial time step size (T).
	21-30	TFAC: Time step multiplier.
	31-40	TMAX: Maximum value of time step allowed (T).

Note: if ITSGN = 0 or 2 (group 3, col. 31-35), TIN and TFAC are not used. Their values may be left blank or set = 0.0

(a-2) Time discretization parameters (5E10.3)

*** Omit unless ITSGN (group 3, Col 31-35) = 3

One record

Col.	1-10	TIMA:	Initial time value (T).
	11-20	TIN:	Initial time step size (T).
	21-30	TMIN:	Minimum allowed time step size (T).
	31-40	TMAX:	Maximum allowed time step size (T).
	41-50	TEND:	Final simulation time (T).

(b) Time values (8E10.3)

*** Omit unless ITSGN (group 3, col. 31-35) = 0

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

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

(c) Time step increments (3E10.3,I5)

*** Omit unless ITSGN = 2.

Number of records = as many as needed.

Each record contains the following information:

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

(d) Nonlinear Scheme Selection Parameters

*** Omit unless ISELSC = 1 (group 4, Col. 56-60) and ITSGN (Group 3, Col. 31-35) = 0, 1 or 2.

(i) Control record (I5,E10.3)

One record.

Col.	1-5	ISWICH:	Parameter indicating whether a switch from the Picard to Newton-Raphson scheme is to be made if convergence difficulty occurs; = 1 if yes, = 0 if no.
	6-15	ENRFAC:	Relaxation factor used to reduce the degree of nonlinearity when convergence difficulty occurs. Suggested value of ENRFAC lies between 0.75 and 1. If no reduction of the degree of nonlinearity is required set ENRFAC = 1. In any case, ENRFAC must not be greater than 1. Note: This option can be used only when the Brooks-Corey relative conductivity function is selected.

(ii) Nonlinear scheme selection records (4I5)

Number of records = as many as needed.

Col.	1-5	ISC:	Nonlinear scheme indicator; = 1 for Newton-Raphson, = 0 for Picard scheme.
	6-10	ITST:	Starting time step number when the specified value of ISC (the selected nonlinear scheme) is to be applied.
	11-15	ITEND:	Ending time step number when the specified value of ISC is to be applied.
	16-20	IPAUSE:	Parameter indicating if this is the last record of subgroup 6d; = 1 if yes, = 0 if no.

7. Default initial values

(a) Dependent variables (2E10.3)

One record.

Col.	1-10	HEADI:	Default initial value of the pressure head (or hydraulic head if INTSPC = 1, or water content if INTSPC=2) (L). Leave blank if dealing with transport simulation only (IMODL = 0).
	11-20	CONCI:	Default initial value of the solute concentration (M/L ³). Leave blank if dealing with flow simulation only (IMODL = 1).

(b) Water saturation (E10.3,I5)

*** Omit if IHYST (group 3, col. 6-10) = 0

One record.

Col.	1-10	SWINT(1):	Default initial value of element saturation.
	11-15	KHYST(1):	Default initial value of the hysteresis index, = -1 if initial condition is drying, = +1 if initial condition is wetting.

Note: If the saturation value is left blank, the saturation will be computed from the initial pressure head value, using parameters for the main drying retention curve if KHYST(1) = -1, or the main wetting curve if KHYST(1) = +1.

8. Element property numbers (16I5)

*** Omit this group if NMAT (group 3, col. 61-65) = 1.

Number of records = NE/16 + (0 or 1).

Col.	1-5 6-10,etc.	IPROP(J): J=1, NE	Material number specification for element number 1 through NE.
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9. Hydraulic properties of soil

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

(a) Saturated property values (7E10.3)

Number of records = NMAT (group 3, col. 61-65).

Col.	1-10	PROP(I,1):	Horizontal component of saturated hydraulic conductivity, K_h (L/T).
	11-20	PROP(I,2):	Vertical component of saturated hydraulic conductivity K_v (L/T). Set $K_v = K_h$ if dealing with isotropic material.
	21-30	PROP(I,3):	Cross component of saturated hydraulic conductivity K_{hv} (L/T). Set $K_{hv} = 0$ unless coordinate axes do not coincide with principal directions of anisotropy.
	31-40	PROP(I,4):	Specific storage, S_s (1/L).
	41-50	PROP(I,5):	Saturated water content, θ_{sat} .
	51-60	PROP(I,6):	Air entry pressure head value, ψ_a (L).
	61-70	SANGLE(I):	Angle (in degrees) of inclination of the surface of the soil material zone. If the zonal surface is horizontal, set this angle to zero. A positive angle corresponds to counterclockwise rotation.

(b) Variable anisotropy parameters (4E10.3)

*** Omit if IANI (group 3, col. 11-15) = 0.

Number of records = NMAT (group 3, col. 46-50).

Col.	1-10	SIGMF(I):	Variance of $\ln K$ -transformed saturated hydraulic conductivity $(L/T)^2$.
	11-20	SIGMAL(I):	Variance of average slope of $\ln [K(\psi)]$ relation.
	21-30	YAMDA(I):	Correlation length normal to stratification (L).

31-40	ANISMX(I):	Maximum allowed anisotropy ratio. Default is 10^7
41-50	AMEAN(I):	Mean slope of the $\ln[k_r(\psi)]$ relation. Will be computed from the specified $k_r(s_w)$ relation if left blank.

10. Soil moisture functional parameters

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

Number of records = NMAT (group 3, col. 46-50, or NMATx2 if IHYST (group 3, col. 6-10) = 1.

(a) Parameters for main drying curve (5E10.3)

Col.	1-10	PROP(I,7):	Residual saturation (S_{wr}) of material number I.
	11-20	PROP(I,8):	Control parameter (n) of the Brooks-Corey relative permeability versus saturation relationship, $k_{rw} = (S_w - S_{wr})^n / (1 - S_{wr})^n$. Set PROP(I,8) = 0 if the van Genuchten k_{rw} versus S_w is to be used instead of the Brooks-Corey relationship.
	21-30	PROP(I,9):	Leading coefficient (α^d) of the van Genuchten saturation versus capillary head relationship (1/L), $(S_w - S_{wr}) = (1 - S_{wr}) / [1 + (\alpha \psi - \psi_a)^{\beta}]^{\gamma}$.
	31-40	PROP(I,10):	Power index (β^d) of the saturation versus capillary head relationship.
	41-50	PROP(I,11):	Power index (γ^d) of the saturation versus capillary head relationship. If PROP(I,11) is left blank, the code then assumes that $\gamma^d = 1 - 1/\beta^d$.

(b) Parameters for main wetting curve (E10.3,10X,3E10.3)

*** Omit if IHYST (group 3, col. 6-10) = 0.

Col.	1-10	PROP(I,12):	Maximum wetting saturation (S_{ws}) of material number I. Default value is $S_{ws} = 1$.
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11-20	blank	
21-30	PROP(I,13):	Leading coefficient (α^w) of the saturation versus capillary head relationship (1/L). Default is $\alpha^w = \alpha^d$.
31-40	PROP(I,14):	Power index (β^w) of the saturation versus capillary head relationship. Default is $\beta^w = \beta^d$.
41-50	PROP(I,15):	Power index (γ^w) of the saturation versus capillary head relationship. If PROP(I,15) is left blank, the code assumes that $\gamma^w = 1-1/\beta^w$.

Note: If a non-hysteretic simulation is performed (IHYST = 0), only group 10a is read. If a hysteretic simulation is performed (IHYST = 1), the parameters for the main drying curve are given in group 10a and the parameters for the main wetting curve are given in group 10b.

11a. Soil physical transport parameters (6E10.3)

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

Number of records = NMAT (group 3, col. 61-65).

Col.	1-10	PROPJ(I,1):	Longitudinal dispersivity, α_L (L).
	11-20	PROPJ(I,2):	Transverse dispersivity, α_T (L).
	21-30	PROPJ(I,3):	Molecular diffusion coefficient, D_{xx}^m (L ² /T).
	31-40	PROPJ(I,4):	Molecular diffusion coefficient, D_{yy}^m (L ² /T).
	41-50	PROPJ(I,5):	Effective porosity, ϕ .
	51-60	PROPJ(I,6):	Bulk density, ρ_B (M/L ³).

11b. Soil-solute transport parameters for single-species simulation (2E10.3)

*** Omit this group if performing flow simulation only (IMODL = 1). Also omit it and proceed to group 11c if multiple-species chained decay simulation is required (ICHAIN = 1).

Number of records = NMAT (group 3, col. 61-65).

- 1-10 RPROP(I,1,1): Decay coefficient, λ (1/T). For a conservative solute species set RPROP(I,1,1) = 0.0. Note $\lambda = \ln 2/t_{1/2}$, where $t_{1/2}$ = half life.
- 11-20 RPROP(I,2,1): Distribution coefficient, k_d (L³/M). Note: the unit for k_d must be the reciprocal of the unit for bulk density. For a unretarded solute species set RPROP(I,2,1) = 0.0.

11c. Soil-solute transport parameters for multispecies simulation

*** Omit this group if IMODL = 1 or ICHAIN = 0.

(i) Control record (2I5)

One record.

Col.	1-5	NSPECI:	Number of solute species that need to be considered.
	6-10	IDSRC:	Parameter indicating if decaying source boundary conditions are to be simulated;
= 1 if yes,
= 0 if no.

(ii) Reaction path indicators

*** Omit if IDSRC = 0.

Flag record (I5)

Col.	1-5	NPATH:	Number of decay chains or reaction paths.
In the case of the straight decay chain, the value of NPATH = 1. |
|------|-----|--------|---|

Follow-up record sets (16I5)

*** Omit if IDSRC = 0.

These record sets are to be repeated NPATH times, for each reaction path.

Col.	1-5	IPATH:	Decay chain or reaction path number.

6-10	NTCOMP:	Number of species components in the chain or path number being considered. For the straight chain case, NTCOMP = NSPECI.
11-15 etc.	KTCOMP(J), J=1, NTCOMP	Sequential component numbers of the transforming components in the decay chain corresponding to the given value of IPATH. For the straight chain case, KTCOMP(J) = J.

(iii) Species transformation data

Number of record sets = NSPECI.

Flag record (2I5)

Col.	1-5	ISP:	Species component number.
	6-10	NPA:	Number of immediate parents.

Follow-up records (4(I5,E10.3))

*** Omit if NPA = 0.

Number of records = NPA (repeat for J=1 through NPA)

Col.	1-5	KPAREN(J):	Species component number of the J-th parent.
	6-15	APAREN(J):	Mass fraction of the J-th parent that decays to species ISP.

(iv) Decay and distribution coefficient data

Number of record sets = NMAT.

Each set contains the following information:

Flag record (2I5)

Col.	1-5	I:	Soil material number
	6-10	IREPET:	Parameter indicating if the following decay and distribution coefficient data are repeated and to be derived from the previous soil material number;

= 1 if yes,
= 0 if no.

First follow-up records (8E10.3)

*** Omit if IREPET = 1.

Col.	1-10	RPROP(I,1,KSP):	Decay coefficient values for species components
	11-20	KSP=1,	1 through NSPECI (T^{-1}).
	etc.	NSPECI	

Second follow-up records (8E10.3)

*** Omit if IREPET = 1.

Col.	1-10	RPROP(I,2,KSP):	Distribution coefficient values for species
	11-20	KSP=1,	components 1 through NSPECI (L^3/M).
	etc.	NSPECI	

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

One record.

Col.	1-5	NROWS:	Number of grid lines parallel to the x-direction.
	6-10	NCOLS:	Number of grid lines parallel to the y-direction.
	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	IXYRED:	Parameter indicating if x and y coordinates of the grid lines are to be input or generated; = 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. = 3 if entire coordinate input is required. (Note: if ICURVL (group 5, col. 71-75)=1, then all nodal coordinates must be specified directly by

the user and IXYRED is automatically set=3; if ICURVL=2, then nodal coordinate values will be read from an external file using the format of group 13c)

36-40 IHORGR: Parameter indicating if the grid corresponds to a horizontal plane, i.e., gravity terms are to be ignored;
 = 0 if no (vertical cross-section);
 = 1 if yes.

13. Grid line and grid coordinates

*** Omit if IXYRED (group 12, col. 31-35) = 0 or 2, or if ICURVL (group 5, col. 71-75) = 2.

(a) Grid line x-coordinates (8F10.4)

*** Omit if IXYRED=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 NCOLS (L).
	11-20	J=1,	
	etc.	NCOLS	

(b) Grid line y-coordinates (8F10.4)

*** Omit if IXYRED=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 NROWS(L).
	11-20	I=1,	
	etc.	NROWS	

(c) Nodal coordinates (8F10.4)

*** Omit unless IXYRED = 3 and ICURVL (group 5, col. 71-75) = 1.

(1) x-coordinates of all nodes

Number of records = NP/8 + 0 or 1 (group 3, col. 41-45).

Col.	1-10	CORD(I,1):	x-coordinates of all nodes in sequential
	11-20	I=1, NP	order.
	etc.		

(2) y-coordinates of all nodes

Number of records = NP/8 + 0 or 1 (group 3, col. 41-45).

Col.	1-10	CORD(I,2):	y-coordinates of all nodes in sequential
	11-20	I=1, NP	order.
	etc.		

14. Mesh generation data (8F10.4)

*** Omit if IXYRED (group 12, col. 31-35) = 1 or 3, or if ICURVL (group 5, col. 71-75) = 2.

(a) Coordinate parameters

One record.

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

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

*** Omit unless IXYRED = 2.

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 (L).
	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; = 0 if no.

Second subset

Each record contains the following information:

Col.	1-10	DELTA _Y :	Spatial increment in the y-direction (L).
	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 $\text{DELTA}_X \cdot (\text{IENDC} - \text{ISTC} + 1)$ must be equal to XO-XSTART; and
- (3) the sum of $\text{DELTA}_Y \cdot (\text{IENDR} - \text{ISTR} + 1)$ must be equal to YO-YSTART.

15. 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. For a general case involving concurrent simulation of variably saturated flow and multispecies transport, the sequential numbers of the dependent variables must be assigned such that the first dependent variable corresponds to pressure head (the dependent variable of the flow equation), and the higher dependent variable numbers correspond to concentrations of species component numbers 1 through the last species in the chain. Species indexing must be arranged according to the order of hierarchy in the chain. This ordering notation for the dependent variables can be easily adapted to simpler cases involving flow or transport simulation only and coupled flow and single-species transport simulation. In order to model solute transport with a decaying source boundary condition, the control parameter ICHAIN (Group 3, Col. 21-25) should be set to ICHAIN=1.

Note that nodes on an infiltration, evaporation or seepage face boundary must not be included in this input group; they are specified in group 24.

(a) Boundary condition control record (5I5)

One record.

Col.	1-5	NBTO:	Number of nodes with steady-state Dirichlet (prescribed head or prescribed concentration) boundary conditions.
	6-10	NDFLUX:	Number of nodes with steady-state prescribed flux boundary conditions. Do not count the time-dependent flux boundary conditions when determining NDFLUX.
	11-15	NBHVAR:	Number of nodes with transient Dirichlet boundary conditions (excluding those corresponding to the decaying source nodes).
	16-20	NBFVAR:	Number of nodes with transient flux boundary conditions (excluding those corresponding to the decaying source nodes).
	21-25	NDCS:	Number of nodes where the decaying source boundary conditions are to be applied. For IMODL = 1 (flow simulation only), the code

automatically sets NDCS = 0. Note: NDCS is ignored unless ICHAIN=1 (Group 3, Col. 21-25).

26-30 NEFREE: Number of elements along free draining lower boundary. Use for flow simulation only.

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

*** Omit this record if NBTO (group 15, col. 1-5)=0.

Number of records = NBTO.

Col.	1-5	NODV(I):	Node number.
	6-10	MDEGB(I):	Dependent variable number.
	11-20	VALVO(I):	Prescribed value of the dependent variable (head or concentration) at the boundary node.

(c) Flux boundary condition data (2I5, 2E10.3)

*** Omit this record if NDFLUX (group 15, col. 6-10) = 0.

Number of records = NDFLUX.

Number of cards = 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.
	6-10	MDEGF(I):	Dependent variable number.
	11-20	FLUXVO(I):	For the flow equation, FLUXVO(I) denotes integrated fluid flux at the boundary node (L^2/T). It is to be left blank if the boundary condition at the node is time dependent. For the transport equation FLUXVO(I) corresponds to the integrated solute flux prescribed at the node (M/LT).
	21-30	QVALV(I):	For the flow equation, QVALV(I) is to be left blank. For the transport equation, QVALV(I)

corresponds to the integrated fluid flux assigned to the boundary node (L^2/T).

(d) Free drainage boundary condition data (16I5)

*** Omit this record if NEFREE (group 15, Col. 26-30) = 0

Number of records = NEFREE/16 + 0 or 1

Col.	1-5	NEF(I):	Sequential <u>element</u> numbers for boundary segment
	6-10	I=1,	where vertical pressure head gradient is zero.
	11-15	NEFREE	

16-I Transient Dirichlet boundary conditions

*** To be omitted if NBHVAR (group 15, col. 11-15) = 0.

Number of record sets = NBHVAR.

Each set contains the following records:

(a) Control record (4I5)

One record.

Col.	1-5	NDHVAR(I):	Node number of a time-dependent head (L) or concentration (M/L^3) boundary node.
	6-10	MDEGBT(I):	Dependent variable number.
	11-15	NTSNDH(I):	Number of control points on the time graph of the boundary condition at the node (Maximum = 100).
	16-20	ITVARH(I):	Parameter indicating the time variation of the prescribed function data; = 0 for continuous variation; = 1 for discontinuous (stepped) variation.

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

Number of records = NTSNDH(I)/8 = 0 or 1 (group 16a, col. 11-15).

Col.	1-10	TMHV(I,J):	Sequential time values (T) corresponding to the
	11-20	J=1,	control points on the time graph depicting
	etc.	NTSNDH(I)	temporal variation of the prescribed dependent
			variable.

(c) Functional value records (8E10.3)

Number of records = $\text{NTSNDH(I)}/8 + 0 \text{ or } 1$ (group 15a, col. 6-10).

Col.	1-10	HVTM(K,J):	Values of the dependent variable corresponding
	11-20	J=1,	to TMHV(I,J).
	etc.	NTSNDH(I)	

16-II Transient flux boundary conditions

*** Omit this record if NBFVAR (group 15, col. 16-20) = 0.

Number of card sets = NBFVAR.

Each set contains the following cards:

(a) Control records (4I5)

One record.

Col.	1-5	NDFVAR(I):	Node number of a time-dependent flux boundary node.
	6-10	MDEGFT(I):	Dependent variable number corresponding to the governing equation being considered.
	11-15	NTSNDF(I):	Number of control points on the time graph of the flux boundary condition at the node (Maximum = 100).
	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 = $\text{NTSNDF(I)}/8 + 0 \text{ or } 1$ (group 16, col. 6-10).

Col.	1-10	TMHF(I,J):	Sequential time values (T) corresponding to the
	11-20	J=1,	control points on the time graph depicting
	etc.	NTSNDF(I)	temporal variation of the flux boundary condition
			at the node.

(c) Flux value cards (8E10.3)

Number of records = NTSNDF(I)/8 + 0 or 1 (group 16, col. 6-10).

Col.	1-10	FVTM(I,J):	Nodal integrated fluid flux values (for flow,
	11-20	J=1,	L^2/T) or solute mass flux values (for
	etc.	NTSNDF(I)	transport, $M/L^3 \times L^2/T$) corresponding to
			TMHF(I,J).

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

*** Omit if dealing with the flow equation. (IMODL = 1, or IMODL = 2 and MDEGFT = 1) (group 3, col. 1-5).

Number of records = NTSNDF(I)/8 + 0 or 1 (group 16, col. 6-10).

Col.	1-10	QVTM(I,J):	Volumetric fluid flux values corresponding to
	11-20	J=1,	TMHF(I,J) (L^2/T).
	etc.	NTSNDF(I)	

17. Decaying source boundary condition data

*** Omit if IMODL = 1 or NDCS = 0.

(a) Decaying source characteristic data

Control record (I5)

Col.	1-5	NDCSRC:	Number of sources to be considered. The correct value of NDCSRC must be greater than zero and less than or equal to NDCS.
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For each source, supply one record set containing the following information:

(1) Leach time data (I5,E10.3)

Col.	1-5	ISC:	Source identification number.
------	-----	------	-------------------------------

6-15 TLDCS(ISC): Leach time duration (T). For a case of continuous leaching source or step release, TLDCS(I) can be left blank or set to a very large value.

(2) Decay coefficient data (8E10.3)

Col.	1-10	SLAMDA(ISC,;	Decay coefficients for species components 1 through NSPECI (1/T).
	11-20	J), J=1,	
	etc.	NSPECI)	

(b) Decaying source node data

One record set for each decaying source node. Each set contains the following information:

Control record (3I5,E10.3)

Col.	1-5	NODCS(I):	Node number.
	6-10	IDCSNO(I):	Decaying source identification number.
	11-15	IBDCS(I):	Boundary condition identifier; = 1 if initial species concentration values are prescribed, = 2 if initial species mass flux values are prescribed.
	16-25	QFLSN(I):	Net integrated fluid flux at the source node (L^2/T).

Initial source-concentration data (8E10.3)

*** Omit if IBDCS(I) = 2.

Col.	1-10	CIDCS(I,ISP):	Initial source concentration values for species components 1 through NSPECI (M/L^3).
	11-20	ISP=1,	
	etc.	NSPECI	

Initial source-flux data (8E10.3)

*** Omit if IBDCS(I) = 1.

Col.	1-10	FMIDCS(I,ISP):	Initial mass flux values (at the source node)
	11-20	ISP=1,	for species components 1 through NSPECI
	etc.	NSPECI	(M/L ³ xL ² /T).

18. Initial nodal value data of dependent variable

This option is not to be used when dealing with multi-species chained transport (ICHAIN = 1).

*** Omit if NONU (group 3, col. 41-45) = 0 or 2. Also omit if NPIN = 0.

Supply these data to the code according to one of the following formats.

(a) Format type 1 (I5, F10.5)

To be used only when NPIN (group 5, col. 11-15) is less than NP (group 3, col. 21-25).

(NOTE: NP = total number of nodes and NPIN = number of nodes for which initial nodal values are to be read).

Number of records to be supplied = NPIN (group 5, col. 11-15).

Col.	1-5	N:	Node number.
	6-15	HINT(N,1):	Initial value of the first dependent variable.
	16-25	HINT(N,2):	Initial value of the second dependent variable.

Note that when the initial water condition for a flow simulation is specified in terms of water content (INTSPC =2), Group 18 is not used, instead the initial data is read in group 21B.

(b) Format type 2 (8E10.3)

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.

19. Default value data (5F10.6, I5)

*** Omit if only flow modeling is required (IMODL (group 3, col. 1-5)=1).

One record.

Col.	1-10	VCX:	Default value of Darcy velocity in the x-direction (L/T).
	11-20	VCY:	Default value of Darcy velocity in the y-direction (L/T).
	21-30	WFAC:	Upstream weighting factor for transport in x-direction. $0 \leq \text{WFAC} \leq 1$. Set to zero or leave blank for no upstream weighting.
	31-40	YFAC:	Upstream weighting factor for transport in y-direction. $0 \leq \text{YFAC} \leq 1$. Set to zero or leave blank for no upstream weighting.
	41-50	SWD:	Default value of initial saturation. Leave blank if not used.
	51-55	IVSTED:	Parameter indicating if the velocity field is steady state; = 1 if yes, = 0 if no.

20. Element Darcy velocity data (2(I5, 2E10.3))

*** This record type is to be omitted unless NVREAD (group 5, col. 1-5) is equal to 1.

Number of records = NE.

Each record contains the following data:

Col.	1-5	I:	Element number.
	6-15	VELX(I):	Value of x-component of Darcy velocity at the element centroid (L/T).
	16-25	VELY(I):	Value of y-component of Darcy velocity at the element centroid (L/T).

21. Element water saturation/water content data

(a) Saturation data for transport simulation (8E10.3)

*** This record type is to be omitted unless variably- saturated transport analysis is to be performed, and NVREAD (group 5, col. 1-5) is equal to 1.

Number of records = $NE/8 + 0$ or 1.

Col.	1-10	SWND(I):	Values of saturation at centroids of elements 1
	11-20	I=1,	through NE.
	etc.	NE	

(b) Initial water content data for flow simulation (8E10.3)

*** This record type is to be omitted unless INTSPC=2 (group 3, col. 16-20) and NONU=1 (Group 3, Col. 66-70).

Number of records = $NE/8 + 0$ or 1

Col.	1-10	SWINT(I):	Values of <u>water content</u> at centroids of elements 1
	11-20	I=1,	through NE.
	etc.	NE	

22. Initial element saturation data for hysteresis simulation

*** Omit if IHYST (group 3, col. 6-10) = 0 or NONU (group 3, col. 51-55) = 0.

(a) Number of elements (I5)

One record.

Col.	1-5	NELS:	Number of elements for which initial saturation values are to be read.
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(b) Saturation and hysteresis data

Format Type 1 (2I5, E10.3)

*** Use if NELS is less than NE.

Number of records = NELS.

Col.	1-5	IL:	Element number.
	6-10	KHYST(IL):	Value of hysteresis index for element IL; = -1 for drying, = +1 for wetting.
	11-20	SWINT(IL):	Saturation value for element IL.

Format Type 2 (16I5 and 8E10.3)

To be used only for a restart run where initial values to be read correspond to the final set of elemental values of the hysteresis index and element water saturation from a previous run. This data can be obtained from file unit 8. The values of the hysteresis index for all elements are read first using 16I5 format, followed by the water content values for all elements using 8E10.3 format.

23. Boundary nodal data

*** This record type is to be omitted if IOUTLT and IMBAL (group 5, col. 46-50) = 0 (flux and/or mass balance calculations are not required).

(a) Control record (I5)

One record.

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

*** Omit if NBOUT (group 21a, col. 1-5) = 0.

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

Col.	1-5	NDOUT(1):	Node numbers of the nodes for which nodal fluid
	6-10	through	flux values are to be computed.
	etc.	NDOUT(NBOUT)	

(c) Nodal numbers for integrated flux computation (8E10.3)

*** Omit this record set if only flow simulation is required (IMODL = 1). Also omit if NVREAD = 2.

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

Col.	1-10	QNDOUT(1):	Nodal values of integrated fluid flux for the
	11-20	through	outlet boundary nodes (L^2/T).
	etc. QNDOUT(NBOUT)		

24. Evaporation, infiltration and seepage data

*** Omit (a) - (c) if NEIEVP (group 3, col. 71-75) = 0.

(a) Control record (4E10.3, I5)

One record.

Col.	1-10	EIMAX:	Maximum value of potential infiltration flux per unit surface area (L/T).
	11-20	PSIMIN:	Minimum value of allowable pressure head at the soil surface (L).
	21-30	EVMAX:	Maximum absolute value of potential evaporation flux per unit surface area (L/T).
	31-40	FRACT:	Fraction of EIMAX and EVMAX to be imposed during the first iteration. Suggested value = 0.1.
			Note that FRACT must be greater than 0 and less than or equal to 1.
	41-45	ITEVT:	Parameter indicating if infiltration flux is transient; = 0 if no, = 1 if yes.
	46-50	INFQP:	Parameter indicating if infiltration flux needs to be printed; = 0 if no, = 1 if yes and detailed check is required for each iteration, = 2 if yes and only total infiltration rate is needed after solution convergence at each time step.

(b) Nodal infiltration or evaporation identification numbers (16I5)

Number of records = NEIEVP/16 + 0 or 1 (group 3, col. 71-75).

Col.	1-5	IELEVP(I):	Sequential number of elements that are subject
	6-10	I=1,	to infiltration or evaporation.
	etc.	NEIEVP	

For those elements that are subject to evaporation, attach negative sign to their sequential elements numbers.

(c) Transient infiltration data

*** Omit if ITEVT (group 24a, col. 41-45) = 0.

(1) Control record (2I5)

One record.

Col.	1-5	NTEVI:	Number of control points on the time graph of the transient infiltration boundary conditions.
	6-10	ITVARE:	Parameter indicating the time variation of the prescribed infiltration data; = 0 for continuous variation; = 1 for stepped variation.

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

Number of records = NTEVI/8 + 0 or 1 (group 24c (1), col. 1-5).

Col.	1-10	TEVIN(I):	Sequential time values corresponding to the control
	11-20	I=1,	points on the time graph depicting temporal
	etc.	NTEVI	variation of infiltration boundary condition (T).

(3) Infiltration value records (8E10.3)

Number of records = NTEVI/8 + 0 or 1 (group 24c (1), col. 1-5)

Col.	1-10	FEVIN(I):	Infiltration flux values corresponding to the time
	11-20	I=1,	values TEVIN(I) (L/T).
	etc.	NTEVI	

(d) Seepage face nodal data

*** Omit if NSEEP (group 4, col. 61-65) = 0.

This record type consists of NSEEP sets. Each set contains the following:

(1) Control record (2I5)

Col.	1-5	NPTOSF(I):	Number of nodes that are expected to lie on seepage-face grid line I.
	6-10	NPSF(I):	Number of nodes that currently lie on the seepage-face grid line I.
	11-15	ISEEQP(I):	Parameter indicating if simulated seepage flux needs to be printed; = 0 if no, = 1 if yes and detailed check is required for each iteration, = 2 if yes and only total seepage rate is needed after solution convergence at each time step.

(2) Nodal seepage-face identification numbers (16I5)

Number of records = NPTOSF(I)/16 + 0 or 1 (group 24d (1), col. 1-5).

Col.	1-5	NDNOSF(I,J):	Sequential global numbers of the nodes expected to
	6-10	J=1,	lie on the seepage-face line I. (See Figure 8.1
	etc.	NPTOSF(I)	for node numbering convention).

25. Plant species data

*** Omit if NPLANT (group 3, col. 76-80) = 0.

(a) Wilting pressure head and potential transpiration (2(I5,2E10.3))

Number of records = NPLANT/2 + 1 or 0 (group 3, col. 76-80).

Col.	1-5	N:	Plant species number.
	6-15	PWILT(N):	Wilting pressure head for species N (L).

Figure 8.1 Sequential node numbers of the nodes expected to lie on the seepage-face line I.

16-25	TPOT(N):	Absolute value of potential transpiration rate
	N=1,	of species N (L/T).
	NPLANT	

(b) Control record (3I5)

One record.

Col.	1-5	NZRDF:	Number of y-coordinate values for which effective root function values are specified.
	6-10	NCOLPL:	Number of vertical nodal columns in the root zone.
	11-15	NEROOT:	Number of finite elements in the root zone.

(c) Depth coordinate records (8E10.3)

Number of records = NZRDF/8 + 1 or 0 (group 24b, col. 1-5).

Col.	1-10	ZRDF(I):	Values of y-coordinate for which root effectiveness
	11-20	I=1,	function values are specified (L).
	etc.	NZRDF	

(d) Effective root function data (8E10.3)

Number of records for each plant = NZRDF/8 + 1 or 0 (group 24b, col. 1-5).

Col.	1-10	RDF(I,J):	Values of effective root function for plant species
	11-20	I=1,	J.
	etc.	NZRDF	

26. Root zone element and node data

*** Omit if NPLANT (group 3, col. 76-80) = 0.

(a) Root zone element data (16I5)

Number of records = NEROOT/16 + 0 or 1 (group 24b, col. 11-15).

Col.	1-5	IEROOT(I):	Sequential numbers of the elements that lie within
	6-10	I=1,	the root zone.
	11-15	NEROOT	
	etc.		

(b) Root zone nodal column data (5I5)

Number of records = NCOLPL (group 24b, col. 6-10).

Col.	1-5	I:	Nodal column number.
	6-10	INDRMN(I):	Lowest nodal sequential number for column I.
	11-15	INDRMX(I):	Highest nodal sequential number for column I.
	16-20	INDICR(I):	Nodal number increment for column I.
	21-25	IPLCOL(I):	Plant species number for column I.

Note: Elements and nodes that are at the soil surface should not be counted because they contribute only to direct evaporation and not to plant transpiration.

27. Observation node data

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

(a) First input option (16I5)

*** Omit if ICHAIN (group 3, col. 21-25) = 1.

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

Col.	1-5	NNOBS:	Number of nodes for which time history of nodal values of dependent variable(s) is to be recorded.
	6-10 etc.	NDOBS(I): I=1, NNOBS	Node numbers of observation nodes.

(b) Second input option

*** Omit if ICHAIN = 0.

(i) Control record (I5)

Col.	1-5	NNOBS:	Number of nodes for which time history of nodal values of dependent variables is to be recorded.
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(ii) Node number records (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	

(iii) Dependent variable number records (16I5)

Col.	1-5	ISPCNO(I),:	Species component numbers selected
	6-10	I=1,	for the observation nodes.
	etc.	NNOBS	

28. Velocity file output time specification data (2E10.3,2I5)

*** Omit unless NVWRIT = 2.

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 onto unit 9 (T).
	11-20	DTVOP:	Time increment for velocity output (T).
	21-25	NDTVOP:	Number of increments with constant value of DTVOP.
	26-30	IPAUSE:	Parameter indicating if this is the last record in group 28; = 1 if yes, = 0 if no.

8.4 INPUT PREPARATION CHECKLIST

To facilitate the preparation of input data for water flow and solute transport simulations, four checklists are provided in Tables 8.1-8.4, respectively. These checklists should be used as a means for echo checking of the input data file (unit number 5).

Table 8.1. Checklist for Water Flow Simulation by VAM2D.

- 1. If there is only one set of material properties specified for the flow system, omit record group 8.**
- 2. If boundary conditions are invariant with time, omit record group 16 and 17.**
- 3. If initial conditions are uniform, omit record group 18.**
- 4. Make sure that the setting of certain control parameters is performed as depicted in Table 8.3.**
- 5. If time step values are to be automatically generated in VAM2D ($ITSGN = 1, 2$ or 3), omit record group 6b.**

Table 8.2. Checklist for Solute Transport Simulation by VAM2D.

1. Omit record group 9 and 10.
2. If there is only one set of material properties specified for the system, omit record group 11.
3. If boundary conditions are invariant with time, omit record group 16 and 17.
4. If initial conditions are uniform, omit record group 18.
5. Make sure that the setting of certain control parameters is performed as depicted in Table 8.4.
6. If time step values are to be automatically generated in VAM2D ($ITSGN = 1$ or 2), omit record group 6b.

Table 8.3. Control Parameters Used by VAM2D in Flow Simulation.

GROUP	COLUMN	VARIABLE	SET VALUE
3	1-5	IMODL	= 1
	6-10	IHYST	= 0 for non-hysteretic soil moisture properties = 1 for hysteretic soil moisture properties
	11-15	IANI	= 0 if variable anisotropy is not to be simulated = 1 if variable anisotropy is to be included in simulation
	16-20	INTSPC	= 0 (for fully-saturated flow) = 0 or 1 (for variably-saturated flow)
	26-30	ISSTA	= 0 if transient analysis is to be performed = 1 if steady state solution is desired
4	11-15	NITMAX	= 1 (for fully-saturated flow), or ≈ 10 (for variably-saturated flow)
	21-25	ILUMP	= 0 for consistent storage matrix = 1 for lumped storage matrix (recommended)
	46-50	IUPSTR	= 0 if upstream weighting of relative permeability is not to be performed = 1 if upstream weighting of relative permeability is desired
5	1 - 5	NVREAD	= 0

Table 8.4. Control Parameter Values Used by VAM2D in the Transport Simulations.

GROUP	COLUMN	VARIABLE	SET VALUE
3	1-5	IMODL	= 0
	21-25	ICHAIN	= 0 if chained decay reaction do not occur = 1 if chained decay reactions are to be simulated (set ICHAIN = 0 for conservative transport simulation)
4	6-10	INEWT	= 0
	11-15	NITMAX	= 1
	16-20	IRESOL	= 0
	21-25	ILUMP	= 0
	26-35	HTOL	= 0.
5	26-30	NVPR	= 0

9 OUTPUT

9.1 GENERAL CONSIDERATIONS

The primary output file from VAM2D 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 velocities and saturation.
- Listing of user-supplied data pertaining to the nonzero flux nodes and flux values.
- Listing of element numbers and centroidal coordinates.
- Listing of information pertaining to convergence of the nonlinear flow solution at each time step.
- Listing of node numbers and values of head or concentration computed by the code. This listing is given for every user-specified time value or time step interval.
- Listing of element numbers and water saturation values for the elements that became unsaturated. This listing is given for every user-specified time value or time step interval.
- Listing of element numbers and the x and y components of Darcy velocity. This listing is given for every user-specified time value or time step interval.

9.2 OUTPUT CONTROL

Output streams are controlled by several control parameters, the values of which must be supplied to the code. Table 9.1 provides a summary of the procedures used to control

various categories of output. The user should decide how much printed output is really needed for the problem simulated. For example, the mesh data and the boundary conditions are normally not needed in the restart run of the same problem.

Table 9.1. Output Control Parameters for File Number 6.

CONTROL PARAMETER	VALUE	MEANING
IPRD	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	Print computed values of head and/or concentration (depending on type of simulation). The output is printed either at every n-th time step or at specific, user-specified time values depending on the value of control parameter NPRCON.
NVPR	n	Print computed values of Darcy velocity and water saturation at the element centroids. The output is printed either at every n-th time step or at specific, user-specified time values, depending on the value of control parameter NPRCON.
NPLOT		Create auxiliary plot output files on units 10 and 11. Output to these files is written at the same time values or time steps as used with the NSTEP and NVPR output.

NOTE: Values of IPRD, NSTEP, NPLOT, and NVPR are read from the data input file described in Section 8.2.

10 INPUT AND OUTPUT FOR FOUR TEST PROBLEMS

10.1 GENERAL CONSIDERATIONS

To demonstrate the utility of the code, input data and computer output from four test problems are provided. The first problem was chosen to demonstrate a transient flow simulation. The second problem was chosen to demonstrate a transient transport simulation using the velocity file from the flow run. The third problem was chosen to demonstrate the capability of the code to perform concurrent analysis of flow and transport. The final problem was chosen to demonstrate a transient multi-component transport simulation involving a three-member chain.

10.2 PROBLEM 1: TRANSIENT UNSATURATED FLOW SIMULATION

10.2.1 Input Data

The input data file for this unsaturated flow problem is displayed in Table 10.1. Because the output control parameter $IPRD = 0$, a complete printout of mesh data, as well as initial condition data will be given as part of the printed output. Also evident in this input data is the specification of $IMODL = 1$. There are three layers of different soil materials. Hydraulic properties of soil and soil moisture functional parameters for each material must also be part of the input. The input data also includes sixteen prescribed head boundary conditions, as well as the node numbers of all nonzero flux boundary nodes. Output is selected at every fifth timestep by setting $NSTEP=NVPR=NPLLOT=5$.

10.2.2 Sample Output

The output from the line printer is displayed in Table 10.2. This output, which corresponds to input data in Table 10.1, consists of the following categories of information:

1. Brief summary of control input data and material hydraulic properties.
2. Prescribed boundary condition data.
3. Initial condition data.
4. Maximum bandwidth of the global matrix for the problem.
5. List of observation nodes.
6. Time-step number.

7. Print check information for convergence of the nonlinear iterations.
8. Fluid flux values at the boundary nodes.
9. Node numbers and nodal head values corresponding to the given time value.
10. List of unsaturated elements and centroidal values of water saturation.
11. List of element numbers and corresponding centroidal values of Darcy velocity components.
12. Mass balance information.
13. Observation node information.

Note that only the results for items 10-15 are only provided for timestep 5.

Table 10.1. Input Data for the Two-Dimensional Unsaturated Flow Problem.

TEST	PROBLEM	10.1	(flow only)															GROUP
1	0	0	0	0	0	1	5	256	225	0	0	3	0	0	0	0	0	1
1	0	15	3	1	0.1	5	5	0.0	0	0	0							2
0	1	0	0	1	5	5	1	1	0	0								3
	0.0		0.5		1.0		1.0											4
-100.0		0.0																5
1	1	1	1	1	1	1	2	2	2	2	2	2	3	3	3	1		6
1	1	1	1	1	1	2	2	2	2	2	2	2	3	3	1	1		7
1	1	1	1	1	2	2	2	2	2	2	2	3	3	1	1	1		8
1	1	1	1	1	2	2	2	2	2	2	2	3	3	1	1	1		9
1	1	1	2	2	2	2	2	2	2	3	3	1	1	1	1	1		10
1	1	2	2	2	2	2	2	3	3	1	1	1	1	1	1	1		11
1	2	2	2	2	2	2	2	3	3	1	1	1	1	1	1	1		12
2	2	2	2	2	2	3	3	1	1	1	1	1	1	1	1	2		13
2	2	2	2	3	3	1	1	1	1	1	1	1	1	2	2	2		14
2	2	2	3	3	1	1	1	1	1	1	1	2	2	2	2	2		15
2	2	3	3	1	1	1	1	1	1	2	2	2	2	2	2	2		16
3	3	1	1	1	1	1	1	1	2	2	2	2	2	2	2	3		17
3																		18
0.350E03	0.350E03	0.000E00	0.000E00	0.410E00	0.000E00													19
2.500E01	2.500E01	0.000E00	0.000E00	0.430E00	0.000E00													20
1.080E01	1.080E01	0.000E00	0.000E00	0.450E00	0.000E00													21
0.0574	1.00	0.124	2.28															22
0.0774	1.00	0.036	1.56															23
0.0675	1.00	0.020	1.41															24
16	16	5.0	10.0	1														25
0.0	2.5	5.0	7.5	10.0	12.5	15.0	17.5											26
20.0	22.5	25.0	30.0	35.0	40.0	45.0	50.0											27
0.0	10.0	20.0	30.0	40.0	50.0	55.0	60.0											28
65.0	70.0	75.0	80.0	85.0	90.0	95.0	100.0											29
16	0	0	16															30
1	1	-100.0																31
17	1	-100.0																32
33	1	-100.0																33
49	1	-100.0																34
65	1	-100.0																35
81	1	-100.0																36
97	1	-100.0																37
113	1	-100.0																38
129	1	-100.0																39
145	1	-100.0																40
161	1	-100.0																41
177	1	-100.0																42
193	1	-100.0																43
209	1	-100.0																44
225	1	-100.0																45
241	1	-100.0																46
16	1	6																47
0.0	1.0	2.0	3.0	4.0	50.0													48
0.0	12.5	10.0	0.0	0.0	0.0													49
32	1	6																50
0.0	1.0	2.0	3.0	4.0	50.0													51
0.0	25.0	20.0	0.0	0.0	0.0													52
48	1	6																53
0.0	1.0	2.0	3.0	4.0	50.0													54
0.0	25.0	20.0	0.0	0.0	0.0													55
64	1	6																56
0.0	1.0	2.0	3.0	4.0	50.0													57
0.0	25.0	20.0	0.0	0.0	0.0													58
80	1	6																59
0.0	1.0	2.0	3.0	4.0	50.0													60
0.0	25.0	20.0	0.0	0.0	0.0													61
96	1	6																62
0.0	1.0	2.0	3.0	4.0	50.0													63
0.0	25.0	20.0	0.0	0.0	0.0													64
112	1	6																65

10-4

Table 10.2. Output for the Two-Dimensional Unsaturated Flow Problem.

```

*****
                        THIS OUTPUT GENERATED BY VAM2D v. 5.2
                        INPUT FILE NAME = a:tbl10.1
*****

NUMBER OF PROBLEMS TO BE SOLVED = 1

PROBLEM NUMBER: 1

PROBLEM TITLE
-----

TEST PROBLEM 10.1 (flow only)
-----

PROBLEM SPECIFICATION PARAMETERS
-----
MODEL OPTION PARAMETER .....(IMODL) = 1
  NOTE: IMODL = 0 FOR SOLUTE TRANSPORT ONLY
          = 1 FOR WATER FLOW ONLY
          = 2 FOR COUPLED FLOW AND TRANSPORT
HYSTERETIC SOIL MOISTURE (1=YES, 0=NO)....(IHYST) = 0
ANISOTROPIC REL. COND.(1=YES, 0=NO).....(IANI) = 0
CONVERT INITIAL HEAD VALUES(1=YES, 0=NO).(INTSPC) = 0
CHAIN-DECAY REACTIONS(1=YES, 0=NO).....(ICHAIN) = 0
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) = 256
TOTAL NUMBER OF ELEMENTS .....(NE) = 225
SEQUENTIAL NUMBERING INDEX (0=Y, 1=X-DIR) (ISWAP) = 0
AXISYMMETRIC SIMULATION(1=YES, 0=NO)....(IAXSYM) = 0
NUMBER OF POROUS MATRIX MATERIALS .....(NMAT) = 3
INITIAL CONDITION NON-UNIFORMITY INDEX....(NONU) = 0
NUMBER OF INFIL./EVAP. ELEMENTS .....(NEIEVP) = 0
NUMBER PLANT SPECIES .....(NPLANT) = 0

TIME STEPPING AND ITERATION CONTROL PARAMETERS
-----
TIME STEPPING INDEX (0=CNTRL, 1=BCKWD) ... (IKALL) = 1
TYPE OF ITERATION SCHEME (1=NEWT, 0=PICARD) (INEWT) = 0
MAXIMUM NON-LINEAR ITERATIONS .....(NITMAX) = 15
MAXIMUM NUMBER OF TIME STEP REFINEMENTS .(IRESOL) = 3
LUMPING OF ELEMENT MATRIX (1=YES, 0=NO) ..(ILUMP) = 1
ABS. ITERATION TOLERANCE FOR HEAD .....(HTOL) = 0.10000E+00
RELATIVE ITERATION TOLERANCE .....(RELCON) = 0.00000E+00
REL. PERMEABILITY UPSTREAM INDEX .....(IUPSTR) = 0
NONLINEAR ITERATION SELECTION .....(ISELSC) = 0

INPUT / OUTPUT CONTROL PARAMETERS
-----
VELOCITY/SATURATION 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 DATA, 3=NO MESH AND I.C. DATA.....(IPRD) =    0
UNIT 9 OUTPUT OF VEL / SAT (1=YES, 0=NO).(NVWRIT) =    1
VELOCITY PRINTOUT CONTROL INDEX.....(NVPR) =    5
UNIT 10 OUTPUT HEAD/CONC. (0=NONE, N=NTH).(NPLOT) =    5
NODAL VALUE PRINTOUT CONTROL INDEX.....(NSTEP) =    5
OBSERVATION NODE INDEX.....(IOBSND) =    1
MASS BALANCE TO BE PERFORMED (1=YES,0=NO).(IMBAL) =    1
UNIT 8 OUTPUT OF HEAD/CONC (1=YES, 0=NO).(NOWRIT) =    0
PRINT CHECK OPTION INDEX.....(IPRCHK) =    0

```

TEMPORAL DISCRETIZATION DATA

```

-----
INITIAL TIME VALUE ..... (TIMA) = 0.0000E+00
VALUE OF FIRST TIME STEP ..... (TIN) = 0.5000E+00
TIME STEP MULTIPLIER ..... (TFAC) = 0.1000E+01
MAXIMUM TIME STEP SIZE ..... (TMAX) = 0.1000E+01

```

*** LIST OF GENERATED TIME VALUES ***

```

-----
0.500E+00 0.100E+01 0.150E+01 0.200E+01 0.250E+01

```

DEFAULT INITIAL VALUE OF PRESSURE HEAD

```

-----
-0.1000E+03

```

ELEMENT PROPERTY NUMBERS

```

-----
1 1 1 1 1 1 1 2 2 2 2 2 2 3 3 1
1 1 1 1 1 1 2 2 2 2 2 2 3 3 1 1
1 1 1 1 1 2 2 2 2 2 2 3 3 1 1 1
1 1 1 2 2 2 2 2 2 2 3 3 1 1 1 1
1 1 2 2 2 2 2 2 2 3 3 1 1 1 1 1
1 2 2 2 2 2 2 2 3 3 1 1 1 1 1 1
2 2 2 2 2 2 2 3 3 1 1 1 1 1 1 2
2 2 2 2 2 3 3 1 1 1 1 1 1 1 2 2
2 2 2 2 3 3 1 1 1 1 1 1 1 2 2 2
2 2 3 3 1 1 1 1 1 1 1 2 2 2 2 2
2 3 3 1 1 1 1 1 1 1 2 2 2 2 2 2
3 3 1 1 1 1 1 1 1 2 2 2 2 2 2 3
3

```

HYDRAULIC PROPERTIES OF POROUS MEDIA

```

-----
MATERIAL NUMBER: 1 (I)

```

```

X-DIRECTION HYDRAULIC CONDUCTIVITY ... (PROP(1,1)) = 0.3500E+03
Y-DIRECTION HYDRAULIC CONDUCTIVITY ... (PROP(1,2)) = 0.3500E+03
XY-DIRECTION HYDRAULIC CONDUCTIVITY .. (PROP(1,3)) = 0.0000E+00
SPECIFIC STORAGE ..... (PROP(1,4)) = 0.0000E+00
SATURATED WATER CONTENT..... (PROP(1,5)) = 0.4100E+00
AIR-ENTRY PRESSURE HEAD VALUE ..... (PROP(1,6)) = 0.0000E+00

```

```

MATERIAL NUMBER: 2 (I)

```

```

X-DIRECTION HYDRAULIC CONDUCTIVITY ... (PROP(1,1)) = 0.2500E+02
Y-DIRECTION HYDRAULIC CONDUCTIVITY ... (PROP(1,2)) = 0.2500E+02
XY-DIRECTION HYDRAULIC CONDUCTIVITY .. (PROP(1,3)) = 0.0000E+00
SPECIFIC STORAGE ..... (PROP(1,4)) = 0.0000E+00
SATURATED WATER CONTENT..... (PROP(1,5)) = 0.4300E+00
AIR-ENTRY PRESSURE HEAD VALUE ..... (PROP(1,6)) = 0.0000E+00

```

MATERIAL NUMBER: 3 (1)

X-DIRECTION HYDRAULIC CONDUCTIVITY ... (PROP(1,1)) = 0.1080E+02
 Y-DIRECTION HYDRAULIC CONDUCTIVITY ... (PROP(1,2)) = 0.1080E+02
 XY-DIRECTION HYDRAULIC CONDUCTIVITY .. (PROP(1,3)) = 0.0000E+00
 SPECIFIC STORAGE (PROP(1,4)) = 0.0000E+00
 SATURATED WATER CONTENT..... (PROP(1,5)) = 0.4500E+00
 AIR-ENTRY PRESSURE HEAD VALUE (PROP(1,6)) = 0.0000E+00

MATERIAL NUMBER: 1 (1)

RESIDUAL WATER SATURATION (PROP(1,7)) = 0.5740E-01
 POWER INDEX (N) OF K(REL) VS SAT..... (PROP(1,8)) = 0.1000E+01
 (SET N=-1 IF VAN GENUCHTEN REL. REQUIRED)
 COEFF (ALPHA) OF SAT. VS CAPIL. HEAD.. (PROP(1,9)) = 0.1240E+00
 POWER INDEX (BETA) ,, ,, (PROP(1,10))= 0.2280E+01
 POWER INDEX (GAMMA) ,, ,, (PROP(1,11))= 0.5614E+00

MATERIAL NUMBER: 2 (1)

RESIDUAL WATER SATURATION (PROP(1,7)) = 0.7740E-01
 POWER INDEX (N) OF K(REL) VS SAT..... (PROP(1,8)) = 0.1000E+01
 (SET N=-1 IF VAN GENUCHTEN REL. REQUIRED)
 COEFF (ALPHA) OF SAT. VS CAPIL. HEAD.. (PROP(1,9)) = 0.3600E-01
 POWER INDEX (BETA) ,, ,, (PROP(1,10))= 0.1560E+01
 POWER INDEX (GAMMA) ,, ,, (PROP(1,11))= 0.3590E+00

MATERIAL NUMBER: 3 (1)

RESIDUAL WATER SATURATION (PROP(1,7)) = 0.6750E-01
 POWER INDEX (N) OF K(REL) VS SAT..... (PROP(1,8)) = 0.1000E+01
 (SET N=-1 IF VAN GENUCHTEN REL. REQUIRED)
 COEFF (ALPHA) OF SAT. VS CAPIL. HEAD.. (PROP(1,9)) = 0.2000E-01
 POWER INDEX (BETA) ,, ,, (PROP(1,10))= 0.1410E+01
 POWER INDEX (GAMMA) ,, ,, (PROP(1,11))= 0.2908E+00

X-COORDINATES OF GRID LINES

0.00	2.50	5.00	7.50	10.00	12.50	15.00	17.50
20.00	22.50	25.00	30.00	35.00	40.00	45.00	50.00

Y-COORDINATES OF GRID LINES

0.00	10.00	20.00	30.00	40.00	50.00	55.00	60.00
65.00	70.00	75.00	80.00	85.00	90.00	95.00	100.00

*** FINITE-ELEMENT MESH CONNECTIONS ***

(NUMBERING IS COUNTER-CLOCKWISE)

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

25	26	42	43	27	26	27	43	44	28	27	28	44	45	29
28	29	45	46	30	29	30	46	47	31	30	31	47	48	32
31	33	49	50	34	32	34	50	51	35	33	35	51	52	36
34	36	52	53	37	35	37	53	54	38	36	38	54	55	39
37	39	55	56	40	38	40	56	57	41	39	41	57	58	42
40	42	58	59	43	41	43	59	60	44	42	44	60	61	45
43	45	61	62	46	44	46	62	63	47	45	47	63	64	48
46	49	65	66	50	47	50	66	67	51	48	51	67	68	52
49	52	68	69	53	50	53	69	70	54	51	54	70	71	55
52	55	71	72	56	53	56	72	73	57	54	57	73	74	58
55	58	74	75	59	56	59	75	76	60	57	60	76	77	61
58	61	77	78	62	59	62	78	79	63	60	63	79	80	64
61	65	81	82	66	62	66	82	83	67	63	67	83	84	68
64	68	84	85	69	65	69	85	86	70	66	70	86	87	71
67	71	87	88	72	68	72	88	89	73	69	73	89	90	74
70	74	90	91	75	71	75	91	92	76	72	76	92	93	77
73	77	93	94	78	74	78	94	95	79	75	79	95	96	80
76	81	97	98	82	77	82	98	99	83	78	83	99	100	84
79	84	100	101	85	80	85	101	102	86	81	86	102	103	87
82	87	103	104	88	83	88	104	105	89	84	89	105	106	90
85	90	106	107	91	86	91	107	108	92	87	92	108	109	93
88	93	109	110	94	89	94	110	111	95	90	95	111	112	96
91	97	113	114	98	92	98	114	115	99	93	99	115	116	100
94	100	116	117	101	95	101	117	118	102	96	102	118	119	103
97	103	119	120	104	98	104	120	121	105	99	105	121	122	106
100	106	122	123	107	101	107	123	124	108	102	108	124	125	109
103	109	125	126	110	104	110	126	127	111	105	111	127	128	112
106	113	129	130	114	107	114	130	131	115	108	115	131	132	116
109	116	132	133	117	110	117	133	134	118	111	118	134	135	119
112	119	135	136	120	113	120	136	137	121	114	121	137	138	122
115	122	138	139	123	116	123	139	140	124	117	124	140	141	125
118	125	141	142	126	119	126	142	143	127	120	127	143	144	128
121	129	145	146	130	122	130	146	147	131	123	131	147	148	132
124	132	148	149	133	125	133	149	150	134	126	134	150	151	135
127	135	151	152	136	128	136	152	153	137	129	137	153	154	138
130	138	154	155	139	131	139	155	156	140	132	140	156	157	141
133	141	157	158	142	134	142	158	159	143	135	143	159	160	144
136	145	161	162	146	137	146	162	163	147	138	147	163	164	148
139	148	164	165	149	140	149	165	166	150	141	150	166	167	151
142	151	167	168	152	143	152	168	169	153	144	153	169	170	154
145	154	170	171	155	146	155	171	172	156	147	156	172	173	157
148	157	173	174	158	149	158	174	175	159	150	159	175	176	160
151	161	177	178	162	152	162	178	179	163	153	163	179	180	164
154	164	180	181	165	155	165	181	182	166	156	166	182	183	167
157	167	183	184	168	158	168	184	185	169	159	169	185	186	170
160	170	186	187	171	161	171	187	188	172	162	172	188	189	173
163	173	189	190	174	164	174	190	191	175	165	175	191	192	176
166	177	193	194	178	167	178	194	195	179	168	179	195	196	180
169	180	196	197	181	170	181	197	198	182	171	182	198	199	183
172	183	199	200	184	173	184	200	201	185	174	185	201	202	186
175	186	202	203	187	176	187	203	204	188	177	188	204	205	189
178	189	205	206	190	179	190	206	207	191	180	191	207	208	192
181	193	209	210	194	182	194	210	211	195	183	195	211	212	196
184	196	212	213	197	185	197	213	214	198	186	198	214	215	199
187	199	215	216	200	188	200	216	217	201	189	201	217	218	202
190	202	218	219	203	191	203	219	220	204	192	204	220	221	205
193	205	221	222	206	194	206	222	223	207	195	207	223	224	208
196	209	225	226	210	197	210	226	227	211	198	211	227	228	212
199	212	228	229	213	200	213	229	230	214	201	214	230	231	215
202	215	231	232	216	203	216	232	233	217	204	217	233	234	218
205	218	234	235	219	206	219	235	236	220	207	220	236	237	221
208	221	237	238	222	209	222	238	239	223	210	223	239	240	224
211	225	241	242	226	212	226	242	243	227	213	227	243	244	228
214	228	244	245	229	215	229	245	246	230	216	230	246	247	231
217	231	247	248	232	218	232	248	249	233	219	233	249	250	234
220	234	250	251	235	221	235	251	252	236	222	236	252	253	237
223	237	253	254	238	224	238	254	255	239	225	239	255	256	240

*** NODAL COORDINATES ***

NODE	X-COOR.	Y-COOR.	NODE	X-COOR.	Y-COOR.	NODE	X-COOR.	Y-COOR.
1	0.00	0.00	2	0.00	10.00	3	0.00	20.00
4	0.00	30.00	5	0.00	40.00	6	0.00	50.00
7	0.00	55.00	8	0.00	60.00	9	0.00	65.00
10	0.00	70.00	11	0.00	75.00	12	0.00	80.00
13	0.00	85.00	14	0.00	90.00	15	0.00	95.00
16	0.00	100.00	17	2.50	0.00	18	2.50	10.00
19	2.50	20.00	20	2.50	30.00	21	2.50	40.00
22	2.50	50.00	23	2.50	55.00	24	2.50	60.00
25	2.50	65.00	26	2.50	70.00	27	2.50	75.00
28	2.50	80.00	29	2.50	85.00	30	2.50	90.00
31	2.50	95.00	32	2.50	100.00	33	5.00	0.00
34	5.00	10.00	35	5.00	20.00	36	5.00	30.00
37	5.00	40.00	38	5.00	50.00	39	5.00	55.00
40	5.00	60.00	41	5.00	65.00	42	5.00	70.00
43	5.00	75.00	44	5.00	80.00	45	5.00	85.00
46	5.00	90.00	47	5.00	95.00	48	5.00	100.00
49	7.50	0.00	50	7.50	10.00	51	7.50	20.00
52	7.50	30.00	53	7.50	40.00	54	7.50	50.00
55	7.50	55.00	56	7.50	60.00	57	7.50	65.00
58	7.50	70.00	59	7.50	75.00	60	7.50	80.00
61	7.50	85.00	62	7.50	90.00	63	7.50	95.00
64	7.50	100.00	65	10.00	0.00	66	10.00	10.00
67	10.00	20.00	68	10.00	30.00	69	10.00	40.00
70	10.00	50.00	71	10.00	55.00	72	10.00	60.00
73	10.00	65.00	74	10.00	70.00	75	10.00	75.00
76	10.00	80.00	77	10.00	85.00	78	10.00	90.00
79	10.00	95.00	80	10.00	100.00	81	12.50	0.00
82	12.50	10.00	83	12.50	20.00	84	12.50	30.00
85	12.50	40.00	86	12.50	50.00	87	12.50	55.00
88	12.50	60.00	89	12.50	65.00	90	12.50	70.00
91	12.50	75.00	92	12.50	80.00	93	12.50	85.00
94	12.50	90.00	95	12.50	95.00	96	12.50	100.00
97	15.00	0.00	98	15.00	10.00	99	15.00	20.00
100	15.00	30.00	101	15.00	40.00	102	15.00	50.00
103	15.00	55.00	104	15.00	60.00	105	15.00	65.00
106	15.00	70.00	107	15.00	75.00	108	15.00	80.00
109	15.00	85.00	110	15.00	90.00	111	15.00	95.00
112	15.00	100.00	113	17.50	0.00	114	17.50	10.00
115	17.50	20.00	116	17.50	30.00	117	17.50	40.00
118	17.50	50.00	119	17.50	55.00	120	17.50	60.00
121	17.50	65.00	122	17.50	70.00	123	17.50	75.00
124	17.50	80.00	125	17.50	85.00	126	17.50	90.00
127	17.50	95.00	128	17.50	100.00	129	20.00	0.00
130	20.00	10.00	131	20.00	20.00	132	20.00	30.00
133	20.00	40.00	134	20.00	50.00	135	20.00	55.00
136	20.00	60.00	137	20.00	65.00	138	20.00	70.00
139	20.00	75.00	140	20.00	80.00	141	20.00	85.00
142	20.00	90.00	143	20.00	95.00	144	20.00	100.00
145	22.50	0.00	146	22.50	10.00	147	22.50	20.00
148	22.50	30.00	149	22.50	40.00	150	22.50	50.00
151	22.50	55.00	152	22.50	60.00	153	22.50	65.00
154	22.50	70.00	155	22.50	75.00	156	22.50	80.00
157	22.50	85.00	158	22.50	90.00	159	22.50	95.00
160	22.50	100.00	161	25.00	0.00	162	25.00	10.00
163	25.00	20.00	164	25.00	30.00	165	25.00	40.00
166	25.00	50.00	167	25.00	55.00	168	25.00	60.00
169	25.00	65.00	170	25.00	70.00	171	25.00	75.00
172	25.00	80.00	173	25.00	85.00	174	25.00	90.00
175	25.00	95.00	176	25.00	100.00	177	30.00	0.00
178	30.00	10.00	179	30.00	20.00	180	30.00	30.00
181	30.00	40.00	182	30.00	50.00	183	30.00	55.00
184	30.00	60.00	185	30.00	65.00	186	30.00	70.00
187	30.00	75.00	188	30.00	80.00	189	30.00	85.00
190	30.00	90.00	191	30.00	95.00	192	30.00	100.00
193	35.00	0.00	194	35.00	10.00	195	35.00	20.00

196	35.00	30.00	197	35.00	40.00	198	35.00	50.00
199	35.00	55.00	200	35.00	60.00	201	35.00	65.00
202	35.00	70.00	203	35.00	75.00	204	35.00	80.00
205	35.00	85.00	206	35.00	90.00	207	35.00	95.00
208	35.00	100.00	209	40.00	0.00	210	40.00	10.00
211	40.00	20.00	212	40.00	30.00	213	40.00	40.00
214	40.00	50.00	215	40.00	55.00	216	40.00	60.00
217	40.00	65.00	218	40.00	70.00	219	40.00	75.00
220	40.00	80.00	221	40.00	85.00	222	40.00	90.00
223	40.00	95.00	224	40.00	100.00	225	45.00	0.00
226	45.00	10.00	227	45.00	20.00	228	45.00	30.00
229	45.00	40.00	230	45.00	50.00	231	45.00	55.00
232	45.00	60.00	233	45.00	65.00	234	45.00	70.00
235	45.00	75.00	236	45.00	80.00	237	45.00	85.00
238	45.00	90.00	239	45.00	95.00	240	45.00	100.00
241	50.00	0.00	242	50.00	10.00	243	50.00	20.00
244	50.00	30.00	245	50.00	40.00	246	50.00	50.00
247	50.00	55.00	248	50.00	60.00	249	50.00	65.00
250	50.00	70.00	251	50.00	75.00	252	50.00	80.00
253	50.00	85.00	254	50.00	90.00	255	50.00	95.00
256	50.00	100.00						

BOUNDARY CONDITION DATA

NUMBER OF STEADY DIRICHLET NODES (NBTO) = 16
 NUMBER OF STEADY FLUX NODES (NDFLUX) = 0
 NUMBER OF TRANSIENT DIRICHLET NODES (NBHVAR) = 0
 NUMBER OF TRANSIENT FLUX NODES (NBFVAR) = 16

DIRICHLET BOUNDARY CONDITION DATA

INDEX	NODE NUMBER	DEP. VAR. #	PRESCRIBED VALUE
1	1	1	-100.0
2	17	1	-100.0
3	33	1	-100.0
4	49	1	-100.0
5	65	1	-100.0
6	81	1	-100.0
7	97	1	-100.0
8	113	1	-100.0
9	129	1	-100.0
10	145	1	-100.0
11	161	1	-100.0
12	177	1	-100.0
13	193	1	-100.0
14	209	1	-100.0
15	225	1	-100.0
16	241	1	-100.0

TIME DEPENDENT FLUX B. C. FOR
 NODE # 16 DEPENDENT VARIABLE # 1

NUMBER OF CONTROL POINTS IN THE TIME GRAPH = 6
 TEMPORAL VARIATION (0=CONTINUOUS, 1=STEP) = 0

TIME VERSUS PRESCRIBED WATER FLUXES

0.0000E+00	0.0000E+00	1.000	12.50	2.000	10.00
3.000	0.0000E+00	4.000	0.0000E+00	50.00	0.0000E+00

TIME DEPENDENT FLUX B. C. FOR
NODE # 32 DEPENDENT VARIABLE # 1

NUMBER OF CONTROL POINTS IN THE TIME GRAPH = 6
TEMPORAL VARIATION (0=CONTINUOUS, 1=STEP) = 0

TIME VERSUS PRESCRIBED WATER FLUXES

0.0000E+00	0.0000E+00	1.000	25.00	2.000	20.00
3.000	0.0000E+00	4.000	0.0000E+00	50.00	0.0000E+00

TIME DEPENDENT FLUX B. C. FOR
NODE # 48 DEPENDENT VARIABLE # 1

NUMBER OF CONTROL POINTS IN THE TIME GRAPH = 6
TEMPORAL VARIATION (0=CONTINUOUS, 1=STEP) = 0

TIME VERSUS PRESCRIBED WATER FLUXES

0.0000E+00	0.0000E+00	1.000	25.00	2.000	20.00
3.000	0.0000E+00	4.000	0.0000E+00	50.00	0.0000E+00

TIME DEPENDENT FLUX B. C. FOR
NODE # 64 DEPENDENT VARIABLE # 1

NUMBER OF CONTROL POINTS IN THE TIME GRAPH = 6
TEMPORAL VARIATION (0=CONTINUOUS, 1=STEP) = 0

TIME VERSUS PRESCRIBED WATER FLUXES

0.0000E+00	0.0000E+00	1.000	25.00	2.000	20.00
3.000	0.0000E+00	4.000	0.0000E+00	50.00	0.0000E+00

TIME DEPENDENT FLUX B. C. FOR
NODE # 80 DEPENDENT VARIABLE # 1

NUMBER OF CONTROL POINTS IN THE TIME GRAPH = 6
TEMPORAL VARIATION (0=CONTINUOUS, 1=STEP) = 0

TIME VERSUS PRESCRIBED WATER FLUXES

0.0000E+00	0.0000E+00	1.000	25.00	2.000	20.00
3.000	0.0000E+00	4.000	0.0000E+00	50.00	0.0000E+00

TIME DEPENDENT FLUX B. C. FOR
NODE # 96 DEPENDENT VARIABLE # 1

NUMBER OF CONTROL POINTS IN THE TIME GRAPH = 6
TEMPORAL VARIATION (0=CONTINUOUS, 1=STEP) = 0

TIME VERSUS PRESCRIBED WATER FLUXES

0.0000E+00	0.0000E+00	1.000	25.00	2.000	20.00
3.000	0.0000E+00	4.000	0.0000E+00	50.00	0.0000E+00

TIME DEPENDENT FLUX B. C. FOR
 NODE # 112 DEPENDENT VARIABLE # 1

NUMBER OF CONTROL POINTS IN THE TIME GRAPH = 6
 TEMPORAL VARIATION (0=CONTINUOUS, 1=STEP) = 0

TIME VERSUS PRESCRIBED WATER FLUXES

0.0000E+00	0.0000E+00	1.000	25.00	2.000	20.00
3.000	0.0000E+00	4.000	0.0000E+00	50.00	0.0000E+00

TIME DEPENDENT FLUX B. C. FOR
 NODE # 128 DEPENDENT VARIABLE # 1

NUMBER OF CONTROL POINTS IN THE TIME GRAPH = 6
 TEMPORAL VARIATION (0=CONTINUOUS, 1=STEP) = 0

TIME VERSUS PRESCRIBED WATER FLUXES

0.0000E+00	0.0000E+00	1.000	25.00	2.000	20.00
3.000	0.0000E+00	4.000	0.0000E+00	50.00	0.0000E+00

TIME DEPENDENT FLUX B. C. FOR
 NODE # 144 DEPENDENT VARIABLE # 1

NUMBER OF CONTROL POINTS IN THE TIME GRAPH = 6
 TEMPORAL VARIATION (0=CONTINUOUS, 1=STEP) = 0

TIME VERSUS PRESCRIBED WATER FLUXES

0.0000E+00	0.0000E+00	1.000	25.00	2.000	20.00
3.000	0.0000E+00	4.000	0.0000E+00	50.00	0.0000E+00

TIME DEPENDENT FLUX B. C. FOR
 NODE # 160 DEPENDENT VARIABLE # 1

NUMBER OF CONTROL POINTS IN THE TIME GRAPH = 6
 TEMPORAL VARIATION (0=CONTINUOUS, 1=STEP) = 0

TIME VERSUS PRESCRIBED WATER FLUXES

0.0000E+00	0.0000E+00	1.000	25.00	2.000	20.00
3.000	0.0000E+00	4.000	0.0000E+00	50.00	0.0000E+00

TIME DEPENDENT FLUX B. C. FOR
 NODE # 176 DEPENDENT VARIABLE # 1

NUMBER OF CONTROL POINTS IN THE TIME GRAPH = 6
 TEMPORAL VARIATION (0=CONTINUOUS, 1=STEP) = 0

TIME VERSUS PRESCRIBED WATER FLUXES

0.0000E+00	0.0000E+00	1.000	37.50	2.000	30.00
3.000	0.0000E+00	4.000	0.0000E+00	50.00	0.0000E+00

TIME DEPENDENT FLUX B. C. FOR
 NODE # 192 DEPENDENT VARIABLE # 1

NUMBER OF CONTROL POINTS IN THE TIME GRAPH = 6
 TEMPORAL VARIATION (0=CONTINUOUS, 1=STEP) = 0

TIME VERSUS PRESCRIBED WATER FLUXES

0.0000E+00	0.0000E+00	1.000	50.00	2.000	40.00
3.000	0.0000E+00	4.000	0.0000E+00	50.00	0.0000E+00

TIME DEPENDENT FLUX B. C. FOR
 NODE # 208 DEPENDENT VARIABLE # 1

NUMBER OF CONTROL POINTS IN THE TIME GRAPH = 6
 TEMPORAL VARIATION (0=CONTINUOUS, 1=STEP) = 0

TIME VERSUS PRESCRIBED WATER FLUXES

0.0000E+00	0.0000E+00	1.000	50.00	2.000	40.00
3.000	0.0000E+00	4.000	0.0000E+00	50.00	0.0000E+00

TIME DEPENDENT FLUX B. C. FOR
 NODE # 224 DEPENDENT VARIABLE # 1

NUMBER OF CONTROL POINTS IN THE TIME GRAPH = 6
 TEMPORAL VARIATION (0=CONTINUOUS, 1=STEP) = 0

TIME VERSUS PRESCRIBED WATER FLUXES

0.0000E+00	0.0000E+00	1.000	50.00	2.000	40.00
3.000	0.0000E+00	4.000	0.0000E+00	50.00	0.0000E+00

TIME DEPENDENT FLUX B. C. FOR
 NODE # 240 DEPENDENT VARIABLE # 1

NUMBER OF CONTROL POINTS IN THE TIME GRAPH = 6
 TEMPORAL VARIATION (0=CONTINUOUS, 1=STEP) = 0

TIME VERSUS PRESCRIBED WATER FLUXES

0.0000E+00	0.0000E+00	1.000	50.00	2.000	40.00
3.000	0.0000E+00	4.000	0.0000E+00	50.00	0.0000E+00

TIME DEPENDENT FLUX B. C. FOR
 NODE # 256 DEPENDENT VARIABLE # 1

NUMBER OF CONTROL POINTS IN THE TIME GRAPH = 6
 TEMPORAL VARIATION (0=CONTINUOUS, 1=STEP) = 0

TIME VERSUS PRESCRIBED WATER FLUXES

0.0000E+00	0.0000E+00	1.000	25.00	2.000	20.00
3.000	0.0000E+00	4.000	0.0000E+00	50.00	0.0000E+00

LIST OF BOUNDARY NODE NUMBERS:

1 16 17 32 33 48 49 64 65 80 81 96 97 112 113 128
129 144 145 160 161 176 177 192 193 208 209 224 225 240 241 256

----- ACTUAL HALF BAND WIDTH = 17 FULL BANDWIDTH = 35 -----

*** ELEMENT CENTROIDAL COORDINATES ***

ELEMENT	X-COOR.	Y-COOR.	ELEMENT	X-COOR.	Y-COOR.	ELEMENT	X-COOR.	Y-COOR.
1	1.25	5.00	2	1.25	15.00	3	1.25	25.00
4	1.25	35.00	5	1.25	45.00	6	1.25	52.50
7	1.25	57.50	8	1.25	62.50	9	1.25	67.50
10	1.25	72.50	11	1.25	77.50	12	1.25	82.50
13	1.25	87.50	14	1.25	92.50	15	1.25	97.50
16	3.75	5.00	17	3.75	15.00	18	3.75	25.00
19	3.75	35.00	20	3.75	45.00	21	3.75	52.50
22	3.75	57.50	23	3.75	62.50	24	3.75	67.50
25	3.75	72.50	26	3.75	77.50	27	3.75	82.50
28	3.75	87.50	29	3.75	92.50	30	3.75	97.50
31	6.25	5.00	32	6.25	15.00	33	6.25	25.00
34	6.25	35.00	35	6.25	45.00	36	6.25	52.50
37	6.25	57.50	38	6.25	62.50	39	6.25	67.50
40	6.25	72.50	41	6.25	77.50	42	6.25	82.50
43	6.25	87.50	44	6.25	92.50	45	6.25	97.50
46	8.75	5.00	47	8.75	15.00	48	8.75	25.00
49	8.75	35.00	50	8.75	45.00	51	8.75	52.50
52	8.75	57.50	53	8.75	62.50	54	8.75	67.50
55	8.75	72.50	56	8.75	77.50	57	8.75	82.50
58	8.75	87.50	59	8.75	92.50	60	8.75	97.50
61	11.25	5.00	62	11.25	15.00	63	11.25	25.00
64	11.25	35.00	65	11.25	45.00	66	11.25	52.50
67	11.25	57.50	68	11.25	62.50	69	11.25	67.50
70	11.25	72.50	71	11.25	77.50	72	11.25	82.50
73	11.25	87.50	74	11.25	92.50	75	11.25	97.50
76	13.75	5.00	77	13.75	15.00	78	13.75	25.00
79	13.75	35.00	80	13.75	45.00	81	13.75	52.50
82	13.75	57.50	83	13.75	62.50	84	13.75	67.50
85	13.75	72.50	86	13.75	77.50	87	13.75	82.50
88	13.75	87.50	89	13.75	92.50	90	13.75	97.50
91	16.25	5.00	92	16.25	15.00	93	16.25	25.00
94	16.25	35.00	95	16.25	45.00	96	16.25	52.50
97	16.25	57.50	98	16.25	62.50	99	16.25	67.50
100	16.25	72.50	101	16.25	77.50	102	16.25	82.50
103	16.25	87.50	104	16.25	92.50	105	16.25	97.50
106	18.75	5.00	107	18.75	15.00	108	18.75	25.00
109	18.75	35.00	110	18.75	45.00	111	18.75	52.50
112	18.75	57.50	113	18.75	62.50	114	18.75	67.50
115	18.75	72.50	116	18.75	77.50	117	18.75	82.50
118	18.75	87.50	119	18.75	92.50	120	18.75	97.50
121	21.25	5.00	122	21.25	15.00	123	21.25	25.00
124	21.25	35.00	125	21.25	45.00	126	21.25	52.50
127	21.25	57.50	128	21.25	62.50	129	21.25	67.50
130	21.25	72.50	131	21.25	77.50	132	21.25	82.50
133	21.25	87.50	134	21.25	92.50	135	21.25	97.50
136	23.75	5.00	137	23.75	15.00	138	23.75	25.00
139	23.75	35.00	140	23.75	45.00	141	23.75	52.50
142	23.75	57.50	143	23.75	62.50	144	23.75	67.50
145	23.75	72.50	146	23.75	77.50	147	23.75	82.50
148	23.75	87.50	149	23.75	92.50	150	23.75	97.50

151	27.50	5.00	152	27.50	15.00	153	27.50	25.00
154	27.50	35.00	155	27.50	45.00	156	27.50	52.50
157	27.50	57.50	158	27.50	62.50	159	27.50	67.50
160	27.50	72.50	161	27.50	77.50	162	27.50	82.50
163	27.50	87.50	164	27.50	92.50	165	27.50	97.50
166	32.50	5.00	167	32.50	15.00	168	32.50	25.00
169	32.50	35.00	170	32.50	45.00	171	32.50	52.50
172	32.50	57.50	173	32.50	62.50	174	32.50	67.50
175	32.50	72.50	176	32.50	77.50	177	32.50	82.50
178	32.50	87.50	179	32.50	92.50	180	32.50	97.50
181	37.50	5.00	182	37.50	15.00	183	37.50	25.00
184	37.50	35.00	185	37.50	45.00	186	37.50	52.50
187	37.50	57.50	188	37.50	62.50	189	37.50	67.50
190	37.50	72.50	191	37.50	77.50	192	37.50	82.50
193	37.50	87.50	194	37.50	92.50	195	37.50	97.50
196	42.50	5.00	197	42.50	15.00	198	42.50	25.00
199	42.50	35.00	200	42.50	45.00	201	42.50	52.50
202	42.50	57.50	203	42.50	62.50	204	42.50	67.50
205	42.50	72.50	206	42.50	77.50	207	42.50	82.50
208	42.50	87.50	209	42.50	92.50	210	42.50	97.50
211	47.50	5.00	212	47.50	15.00	213	47.50	25.00
214	47.50	35.00	215	47.50	45.00	216	47.50	52.50
217	47.50	57.50	218	47.50	62.50	219	47.50	67.50
220	47.50	72.50	221	47.50	77.50	222	47.50	82.50
223	47.50	87.50	224	47.50	92.50	225	47.50	97.50

LIST OF OBSERVATION NODES

62 126 150 174 222

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

**** ELAPSED SIMULATION TIME : 0.5000 TIME STEP NUMBER : 1 TIME STEP SIZE: 0.500E+00 ****

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM ERROR	NODE NUMBER	RELAXATION FACTOR
1	240	-42.40	256	1.00
2	240	4.440	224	0.933
3	208	0.2076	23	1.00
4	0	-3.3737E-02	48	0.897

SOLUTION IS NOW COMPLETE FOR TARGET TIME STEP NO. 1 NUMBER OF COMPUTATIONAL TIME STEPS PERFORMED = 1

**** ELAPSED SIMULATION TIME : 1.000 TIME STEP NUMBER : 2 TIME STEP SIZE: 0.500E+00 ****

NUMBER OF

ITERATION	NON-CONVERGENT NODES	MAXIMUM ERROR	NODE NUMBER	RELAXATION FACTOR
1	240	50.15	240	1.00
2	224	-9.925	192	0.876
3	112	0.2300	192	0.983
4	0	3.7496E-02	218	1.00

SOLUTION IS NOW COMPLETE FOR TARGET TIME STEP NO. 2 NUMBER OF COMPUTATIONAL TIME STEPS PERFORMED = 1

**** ELAPSED SIMULATION TIME : 1.500 TIME STEP NUMBER : 3 TIME STEP SIZE: 0.500E+00 ****

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM ERROR	NODE NUMBER	RELAXATION FACTOR
1	240	-17.98	240	1.00
2	208	2.344	240	0.917
3	0	-5.5409E-02	16	0.983

SOLUTION IS NOW COMPLETE FOR TARGET TIME STEP NO. 3 NUMBER OF COMPUTATIONAL TIME STEPS PERFORMED = 1

**** ELAPSED SIMULATION TIME : 2.000 TIME STEP NUMBER : 4 TIME STEP SIZE: 0.500E+00 ****

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM ERROR	NODE NUMBER	RELAXATION FACTOR
1	240	-5.342	208	1.00
2	192	0.9519	192	0.888
3	0	2.7004E-02	198	1.00

SOLUTION IS NOW COMPLETE FOR TARGET TIME STEP NO. 4 NUMBER OF COMPUTATIONAL TIME STEPS PERFORMED = 1

**** ELAPSED SIMULATION TIME : 2.500 TIME STEP NUMBER : 5 TIME STEP SIZE: 0.500E+00 ****

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM ERROR	NODE NUMBER	RELAXATION FACTOR
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1	240	-24.66	64	1.00
2	192	1.710	64	0.955
3	0	3.9083E-02	22	1.00

*** NODAL FLUID FLUX VALUES ***

NODE	FLUID FLUX	NODE	FLUID FLUX	NODE	FLUID FLUX	NODE	FLUID FLUX	NODE	FLUID FLUX
1	-6.385	16	5.000	17	-12.77	32	10.00	33	-12.77
48	10.00	49	-12.77	64	10.00	65	-12.77	80	10.00
81	-12.77	96	10.00	97	-12.77	112	10.00	113	-12.77
128	10.00	129	-12.77	144	10.00	145	-12.77	160	10.00
161	-19.16	176	15.00	177	-25.54	192	20.00	193	-25.54
208	20.00	209	-25.54	224	20.00	225	-25.54	240	20.00
241	-12.77	256	10.00						

SUM OF ABOVE FLUX VALUES = -55.408

*** NODAL HEAD VALUES ***

NODE	HEAD VALUE	NODE	HEAD VALUE	NODE	HEAD VALUE	NODE	HEAD VALUE	NODE	HEAD VALUE
1	-100.0	2	-106.2	3	-112.1	4	-117.7	5	-123.1
6	-128.3	7	-130.8	8	-133.2	9	-135.7	10	-138.3
11	-140.9	12	-143.5	13	-146.2	14	-148.9	15	-150.6
16	-152.5	17	-100.0	18	-106.2	19	-112.1	20	-117.7
21	-123.1	22	-128.3	23	-130.8	24	-133.2	25	-135.7
26	-138.3	27	-140.9	28	-143.5	29	-146.2	30	-148.9
31	-150.6	32	-152.5	33	-100.0	34	-106.2	35	-112.1
36	-117.7	37	-123.1	38	-128.3	39	-130.8	40	-133.2
41	-135.7	42	-138.3	43	-140.9	44	-143.5	45	-146.2
46	-148.9	47	-150.6	48	-152.5	49	-100.0	50	-106.2
51	-112.1	52	-117.7	53	-123.1	54	-128.3	55	-130.8
56	-133.2	57	-135.7	58	-138.3	59	-140.9	60	-143.5
61	-146.2	62	-148.9	63	-150.6	64	-152.5	65	-100.0
66	-106.2	67	-112.1	68	-117.7	69	-123.1	70	-128.3
71	-130.8	72	-133.2	73	-135.7	74	-138.3	75	-140.9
76	-143.5	77	-146.2	78	-148.9	79	-150.6	80	-152.5
81	-100.0	82	-106.2	83	-112.1	84	-117.7	85	-123.1
86	-128.3	87	-130.8	88	-133.2	89	-135.7	90	-138.3
91	-140.9	92	-143.5	93	-146.2	94	-148.9	95	-150.6
96	-152.5	97	-100.0	98	-106.2	99	-112.1	100	-117.7
101	-123.1	102	-128.3	103	-130.8	104	-133.2	105	-135.7
106	-138.3	107	-140.9	108	-143.5	109	-146.2	110	-148.9
111	-150.6	112	-152.5	113	-100.0	114	-106.2	115	-112.1
116	-117.7	117	-123.1	118	-128.3	119	-130.8	120	-133.2
121	-135.7	122	-138.3	123	-140.9	124	-143.5	125	-146.2
126	-148.9	127	-150.6	128	-152.5	129	-100.0	130	-106.2
131	-112.1	132	-117.7	133	-123.1	134	-128.3	135	-130.8
136	-133.2	137	-135.7	138	-138.3	139	-140.9	140	-143.5
141	-146.2	142	-148.9	143	-150.6	144	-152.5	145	-100.0
146	-106.2	147	-112.1	148	-117.7	149	-123.1	150	-128.3
151	-130.8	152	-133.2	153	-135.7	154	-138.3	155	-140.9
156	-143.5	157	-146.2	158	-148.9	159	-150.6	160	-152.5
161	-100.0	162	-106.2	163	-112.1	164	-117.7	165	-123.1
166	-128.3	167	-130.8	168	-133.2	169	-135.7	170	-138.3
171	-140.9	172	-143.5	173	-146.2	174	-148.9	175	-150.6
176	-152.5	177	-100.0	178	-106.2	179	-112.1	180	-117.7
181	-123.1	182	-128.3	183	-130.8	184	-133.2	185	-135.7
186	-138.3	187	-140.9	188	-143.5	189	-146.2	190	-148.9

191	-150.6	192	-152.5	193	-100.0	194	-106.2	195	-112.1
196	-117.7	197	-123.1	198	-128.3	199	-130.8	200	-133.2
201	-135.7	202	-138.3	203	-140.9	204	-143.5	205	-146.2
206	-148.9	207	-150.6	208	-152.5	209	-100.0	210	-106.2
211	-112.1	212	-117.7	213	-123.1	214	-128.3	215	-130.8
216	-133.2	217	-135.7	218	-138.3	219	-140.9	220	-143.5
221	-146.2	222	-148.9	223	-150.6	224	-152.5	225	-100.0
226	-106.2	227	-112.1	228	-117.7	229	-123.1	230	-128.3
231	-130.8	232	-133.2	233	-135.7	234	-138.3	235	-140.9
236	-143.5	237	-146.2	238	-148.9	239	-150.6	240	-152.5
241	-100.0	242	-106.2	243	-112.1	244	-117.7	245	-123.1
246	-128.3	247	-130.8	248	-133.2	249	-135.7	250	-138.3
251	-140.9	252	-143.5	253	-146.2	254	-148.9	255	-150.6
256	-152.5								

*** LIST OF PARTIALLY SATURATED ELEMENTS ***

ELEM.	SAT. VALUE	ELEM.	SAT. VALUE	ELEM.	SAT. VALUE	ELEM.	SAT. VALUE	ELEM.	SAT. VALUE
1	0.0935	2	0.0910	3	0.0888	4	0.0870	5	0.0854
6	0.0844	7	0.0837	8	0.4478	9	0.4442	10	0.4407
11	0.4373	12	0.4338	13	0.4304	14	0.6298	15	0.6275
16	0.0935	17	0.0910	18	0.0888	19	0.0870	20	0.0854
21	0.0844	22	0.0837	23	0.4478	24	0.4442	25	0.4407
26	0.4373	27	0.4338	28	0.4304	29	0.6298	30	0.6275
31	0.0935	32	0.0910	33	0.0888	34	0.0870	35	0.0854
36	0.0844	37	0.0837	38	0.4478	39	0.4442	40	0.4407
41	0.4373	42	0.4338	43	0.4304	44	0.6298	45	0.6275
46	0.0935	47	0.0910	48	0.0888	49	0.0870	50	0.0854
51	0.0844	52	0.0837	53	0.4478	54	0.4442	55	0.4407
56	0.4373	57	0.4338	58	0.4304	59	0.6298	60	0.6275
61	0.0935	62	0.0910	63	0.0888	64	0.0870	65	0.0854
66	0.0844	67	0.0837	68	0.4478	69	0.4442	70	0.4407
71	0.4373	72	0.4338	73	0.4304	74	0.6298	75	0.6275
76	0.0935	77	0.0910	78	0.0888	79	0.0870	80	0.0854
81	0.0844	82	0.0837	83	0.4478	84	0.4442	85	0.4407
86	0.4373	87	0.4338	88	0.4304	89	0.6298	90	0.6275
91	0.0935	92	0.0910	93	0.0888	94	0.0870	95	0.0854
96	0.0844	97	0.0837	98	0.4478	99	0.4442	100	0.4407
101	0.4373	102	0.4338	103	0.4304	104	0.6298	105	0.6275
106	0.0935	107	0.0910	108	0.0888	109	0.0870	110	0.0854
111	0.0844	112	0.0837	113	0.4478	114	0.4442	115	0.4407
116	0.4373	117	0.4338	118	0.4304	119	0.6298	120	0.6275
121	0.0935	122	0.0910	123	0.0888	124	0.0870	125	0.0854
126	0.0844	127	0.0837	128	0.4478	129	0.4442	130	0.4407
131	0.4373	132	0.4338	133	0.4304	134	0.6298	135	0.6275
136	0.0935	137	0.0910	138	0.0888	139	0.0870	140	0.0854
141	0.0844	142	0.0837	143	0.4478	144	0.4442	145	0.4407
146	0.4373	147	0.4338	148	0.4304	149	0.6298	150	0.6275
151	0.0935	152	0.0910	153	0.0888	154	0.0870	155	0.0854
156	0.0844	157	0.0837	158	0.4478	159	0.4442	160	0.4407
161	0.4373	162	0.4338	163	0.4304	164	0.6298	165	0.6275
166	0.0935	167	0.0910	168	0.0888	169	0.0870	170	0.0854
171	0.0844	172	0.0837	173	0.4478	174	0.4442	175	0.4407
176	0.4373	177	0.4338	178	0.4304	179	0.6298	180	0.6275
181	0.0935	182	0.0910	183	0.0888	184	0.0870	185	0.0854
186	0.0844	187	0.0837	188	0.4478	189	0.4442	190	0.4407
191	0.4373	192	0.4338	193	0.4304	194	0.6298	195	0.6275
196	0.0935	197	0.0910	198	0.0888	199	0.0870	200	0.0854
201	0.0844	202	0.0837	203	0.4478	204	0.4442	205	0.4407
206	0.4373	207	0.4338	208	0.4304	209	0.6298	210	0.6275
211	0.0935	212	0.0910	213	0.0888	214	0.0870	215	0.0854
216	0.0844	217	0.0837	218	0.4478	219	0.4442	220	0.4407
221	0.4373	222	0.4338	223	0.4304	224	0.6298	225	0.6275

*** ELEMENTAL FLUID VELOCITY ***

ELEMENT	X-VELOCITY	Y-VELOCITY	ELEMENT	X-VELOCITY	Y-VELOCITY	ELEMENT	X-VELOCITY	Y-VELOCITY
1	0.000E+00	-5.11	2	0.000E+00	-5.10	3	6.633E-14	-5.09
4	6.246E-14	-5.07	5	0.000E+00	-5.04	6	0.000E+00	-5.02
7	0.000E+00	-5.01	8	5.705E-14	-4.95	9	1.130E-13	-4.85
10	5.596E-14	-4.75	11	0.000E+00	-4.63	12	0.000E+00	-4.51
13	0.000E+00	-4.38	14	3.702E-14	-4.25	15	3.687E-14	-4.09
16	-7.622E-14	-5.11	17	-7.085E-14	-5.10	18	1.327E-13	-5.09
19	1.249E-13	-5.07	20	-5.913E-14	-5.04	21	-1.138E-13	-5.02
22	-1.111E-13	-5.01	23	-5.705E-14	-4.95	24	0.000E+00	-4.85
25	5.596E-14	-4.75	26	5.543E-14	-4.63	27	-5.490E-14	-4.51
28	5.438E-14	-4.38	29	1.111E-13	-4.25	30	1.106E-13	-4.09
31	0.000E+00	-5.11	32	2.126E-13	-5.10	33	2.653E-13	-5.09
34	1.249E-13	-5.07	35	5.913E-14	-5.04	36	0.000E+00	-5.02
37	0.000E+00	-5.01	38	-1.141E-13	-4.95	39	-1.130E-13	-4.85
40	5.596E-14	-4.75	41	0.000E+00	-4.63	42	0.000E+00	-4.51
43	5.438E-14	-4.38	44	3.702E-14	-4.25	45	0.000E+00	-4.09
46	7.622E-14	-5.11	47	1.417E-13	-5.10	48	1.327E-13	-5.09
49	2.498E-13	-5.07	50	5.913E-14	-5.04	51	-1.138E-13	-5.02
52	-1.666E-13	-5.01	53	-1.712E-13	-4.95	54	-5.650E-14	-4.85
55	-1.119E-13	-4.75	56	-5.543E-14	-4.63	57	5.490E-14	-4.51
58	1.631E-13	-4.38	59	1.851E-13	-4.25	60	1.475E-13	-4.09
61	1.524E-13	-5.11	62	2.126E-13	-5.10	63	1.327E-13	-5.09
64	1.249E-13	-5.07	65	5.913E-14	-5.04	66	-5.688E-14	-5.02
67	-2.221E-13	-5.01	68	-1.712E-13	-4.95	69	-2.260E-13	-4.85
70	-1.119E-13	-4.75	71	1.109E-13	-4.63	72	1.098E-13	-4.51
73	1.631E-13	-4.38	74	1.111E-13	-4.25	75	1.475E-13	-4.09
76	2.287E-13	-5.11	77	3.543E-13	-5.10	78	2.653E-13	-5.09
79	1.249E-13	-5.07	80	1.183E-13	-5.04	81	0.000E+00	-5.02
82	-1.666E-13	-5.01	83	-1.712E-13	-4.95	84	-5.650E-14	-4.85
85	0.000E+00	-4.75	86	5.543E-14	-4.63	87	1.647E-13	-4.51
88	1.088E-13	-4.38	89	7.403E-14	-4.25	90	1.106E-13	-4.09
91	2.287E-13	-5.11	92	3.543E-13	-5.10	93	2.653E-13	-5.09
94	1.249E-13	-5.07	95	1.183E-13	-5.04	96	1.138E-13	-5.02
97	0.000E+00	-5.01	98	-2.282E-13	-4.95	99	-1.695E-13	-4.85
100	5.596E-14	-4.75	101	1.109E-13	-4.63	102	0.000E+00	-4.51
103	-1.088E-13	-4.38	104	1.111E-13	-4.25	105	2.212E-13	-4.09
106	1.524E-13	-5.11	107	2.834E-13	-5.10	108	1.327E-13	-5.09
109	0.000E+00	-5.07	110	1.183E-13	-5.04	111	2.275E-13	-5.02
112	5.553E-14	-5.01	113	-5.705E-14	-4.95	114	0.000E+00	-4.85
115	0.000E+00	-4.75	116	0.000E+00	-4.63	117	0.000E+00	-4.51
118	0.000E+00	-4.38	119	-3.702E-14	-4.25	120	3.687E-14	-4.09
121	0.000E+00	-5.11	122	2.126E-13	-5.10	123	2.653E-13	-5.09
124	1.249E-13	-5.07	125	1.183E-13	-5.04	126	1.706E-13	-5.02
127	5.553E-14	-5.01	128	-5.705E-14	-4.95	129	-1.130E-13	-4.85
130	-1.679E-13	-4.75	131	-1.663E-13	-4.63	132	-1.098E-13	-4.51
133	-5.438E-14	-4.38	134	7.403E-14	-4.25	135	7.374E-14	-4.09
136	0.000E+00	-5.11	137	1.417E-13	-5.10	138	2.653E-13	-5.09
139	1.249E-13	-5.07	140	0.000E+00	-5.04	141	5.688E-14	-5.02
142	1.111E-13	-5.01	143	1.141E-13	-4.95	144	-5.650E-14	-4.85
145	-1.679E-13	-4.75	146	-1.109E-13	-4.63	147	-5.490E-14	-4.51
148	0.000E+00	-4.38	149	-3.702E-14	-4.25	150	0.000E+00	-4.09
151	3.811E-14	-5.11	152	1.363E-13	-5.10	153	1.990E-13	-5.09
154	9.369E-14	-5.07	155	-5.913E-14	-5.04	156	-2.844E-14	-5.02
157	1.388E-13	-5.01	158	1.426E-13	-4.95	159	0.000E+00	-4.85
160	-1.679E-13	-4.75	161	-1.386E-13	-4.63	162	8.235E-14	-4.51
163	8.156E-14	-4.38	164	-1.851E-14	-4.25	165	-7.374E-14	-4.09
166	-3.811E-14	-5.11	167	3.543E-14	-5.10	168	6.633E-14	-5.09
169	3.123E-14	-5.07	170	2.56E-14	-5.04	171	0.000E+00	-5.02
172	-2.776E-14	-5.01	173	-5.705E-14	-4.95	174	-1.130E-13	-4.85
175	-2.798E-14	-4.75	176	0.000E+00	-4.63	177	-1.098E-13	-4.51
178	-1.359E-13	-4.38	179	-5.553E-14	-4.25	180	0.000E+00	-4.09
181	7.622E-14	-5.11	182	7.085E-14	-5.10	183	3.316E-14	-5.09
184	3.123E-14	-5.07	185	2.956E-14	-5.04	186	0.000E+00	-5.02
187	-5.553E-14	-5.01	188	-1.997E-13	-4.95	189	-2.260E-13	-4.85
190	-1.959E-13	-4.75	191	-1.386E-13	-4.63	192	-1.098E-13	-4.51
193	-5.438E-14	-4.38	194	0.000E+00	-4.25	195	0.000E+00	-4.09
196	0.000E+00	-5.11	197	0.000E+00	-5.10	198	3.316E-14	-5.09
199	3.123E-14	-5.07	200	-2.956E-14	-5.04	201	-5.688E-14	-5.02
202	-8.329E-14	-5.01	203	-5.705E-14	-4.95	204	-2.825E-14	-4.85
205	-5.596E-14	-4.75	206	-8.314E-14	-4.63	207	-2.745E-14	-4.51

208	-2.719E-14	-4.38	209	-1.851E-14	-4.25	210	0.000E+00	-4.09
211	0.000E+00	-5.11	212	0.000E+00	-5.10	213	0.000E+00	-5.09
214	3.123E-14	-5.07	215	-2.956E-14	-5.04	216	-8.532E-14	-5.02
217	-2.776E-14	-5.01	218	5.705E-14	-4.95	219	5.650E-14	-4.85
220	2.798E-14	-4.75	221	5.543E-14	-4.63	222	0.000E+00	-4.51
223	-8.156E-14	-4.38	224	-7.403E-14	-4.25	225	-3.687E-14	-4.09

SOLUTION IS NOW COMPLETE FOR TARGET TIME STEP NO. 5 NUMBER OF COMPUTATIONAL TIME STEPS PERFORMED = 1

*** VOLUMETRIC FLOW BALANCE INFORMATION AT TIME = 0.2500E+01***

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

NET FLOW RATE DUE TO BOUNDARY FLUX AND SINKS -55.408
 RATE OF FLUID ACCUMULATION -58.559
 MASS BALANCE ERROR 3.1501
 NORMALIZED MASS BALANCE ERROR 6.12901E-03
 CUMULATIVE FLUID STORAGE -73.844

*** OBSERVATION NODE INFORMATION ***

NODAL VALUES OF DEPENDENT VARIABLE OVER TIME

OBSERVED NODE NUMBER: 62

TIME	HEAD VALUE	TIME	HEAD VALUE	TIME	HEAD VALUE	TIME	HEAD VALUE
0.5000E+00	-0.1360E+03	0.1000E+01	-0.1195E+03	0.1500E+01	-0.1210E+03	0.2000E+01	-0.1262E+03
0.2500E+01	-0.1489E+03						

OBSERVED NODE NUMBER: 126

TIME	HEAD VALUE	TIME	HEAD VALUE	TIME	HEAD VALUE	TIME	HEAD VALUE
0.5000E+00	-0.1360E+03	0.1000E+01	-0.1195E+03	0.1500E+01	-0.1210E+03	0.2000E+01	-0.1262E+03
0.2500E+01	-0.1489E+03						

OBSERVED NODE NUMBER: 150

TIME	HEAD VALUE	TIME	HEAD VALUE	TIME	HEAD VALUE	TIME	HEAD VALUE
0.5000E+00	-0.1209E+03	0.1000E+01	-0.1139E+03	0.1500E+01	-0.1142E+03	0.2000E+01	-0.1168E+03
0.2500E+01	-0.1283E+03						

OBSERVED NODE NUMBER: 174

TIME	HEAD VALUE	TIME	HEAD VALUE	TIME	HEAD VALUE	TIME	HEAD VALUE
0.5000E+00	-0.1360E+03	0.1000E+01	-0.1195E+03	0.1500E+01	-0.1210E+03	0.2000E+01	-0.1262E+03
0.2500E+01	-0.1489E+03						

OBSERVED NODE NUMBER: 222

TIME	HEAD VALUE	TIME	HEAD VALUE	TIME	HEAD VALUE	TIME	HEAD VALUE
0.5000E+00	-0.1360E+03	0.1000E+01	-0.1195E+03	0.1500E+01	-0.1210E+03	0.2000E+01	-0.1262E+03
0.2500E+01	-0.1489E+03						

***** VAM2D HAS FULLY EXECUTED *****

10.3 PROBLEM 2: TRANSIENT TRANSPORT SIMULATION

10.3.1 Input Data

The input data file for this sample transport problem is presented in Table 10.3. Note that the modeling option parameter $IMODL = 0$. Because the output control parameter $IPRD$ is set equal to 2, the mesh data DOES NOT appear in the printed output. Also evident in the depicted input data is the specification of $NVREAD = 2$. This means that data pertaining to Darcy velocity and water saturation values must be supplied to the code from a separate data file in TAPE9, which was written during the solution of the previous flow problem. Finally, the input data shown in Table 10.3 also contains sixteen prescribed concentration boundary conditions, as well as node numbers of all non-zero flux boundary nodes. Output options are the same as in the first example problem.

10.3.2 Sample Output

Output of the transport calculation is displayed in Table 10.4. This output consists of the following categories of information:

1. Brief summary of control input data and material transport properties.
2. Prescribed boundary condition data.
3. Default value of velocities and upstream weighting factors.
4. Maximum bandwidth of the global matrix.
5. List of observation nodes.
6. Time step number.
7. Element velocities, water saturation, nodal storage, and flux values that were read from file number 9.
8. Mass balance information.
9. Node numbers and concentration values corresponding to the given time value.
10. Observation node information.

Note that information in categories 9 through 11 is printed for the 5-th timestep only.

Table 10.3. Input Data for the Two-Dimensional Solute Transport Problem.

1 TEST PROBLEM	2 2	(TRANSPORT ONLY)														GROUP 1
0	0	0	0	0	0	1	5	256	225	0	0	3	0	0	0	GROUP 2
1	0	10	1	1	0.1			1.0								GROUP 3
2	1	0	2	0	5	5	5	1	1	0	0					GROUP 4
	0.0		0.5		1.0		1.0									GROUP 5
-100.0			0.0													GROUP 6
1	1	1	1	1	1	1	2	2	2	2	2	2	3	3	1	GROUP 7
1	1	1	1	1	1	1	2	2	2	2	2	3	3	1	1	GROUP 8
1	1	1	1	1	1	2	2	2	2	2	3	3	1	1	1	..
1	1	1	1	1	2	2	2	2	2	3	3	1	1	1	1	..
1	1	1	1	2	2	2	2	2	2	3	3	1	1	1	1	..
1	1	1	2	2	2	2	2	2	3	3	1	1	1	1	1	..
1	1	2	2	2	2	2	2	3	3	1	1	1	1	1	1	..
2	2	2	2	2	2	3	3	1	1	1	1	1	1	1	2	..
2	2	2	2	2	3	3	1	1	1	1	1	1	1	2	2	..
2	2	2	3	3	1	1	1	1	1	1	2	2	2	2	2	..
2	2	3	3	1	1	1	1	1	1	2	2	2	2	2	2	..
3	3	1	1	1	1	1	1	1	2	2	2	2	2	2	3	..
3																..
	2.0		2.0		0.0		0.0		0.41		1.65					GROUP 11A
	2.0		2.0		0.0		0.0		0.43		1.55					..
	2.0		2.0		0.0		0.0		0.45		1.50					..
	0.0		0.0													GROUP 11B
	0.0		0.0													..
	0.0		0.0													..
16	16		5.0		10.0	1										GROUP 12
	0.0		2.5		5.0		7.5		10.0		12.5		15.0		17.5	GROUP 13
	20.0		22.5		25.0		30.0		35.0		40.0		45.0		50.0	..
	0.0		10.0		20.0		30.0		40.0		50.0		55.0		60.0	..
	65.0		70.0		75.0		80.0		85.0		90.0		95.0		100.0	..
16	0	0	16													GROUP 15A
16	1		1.0													GROUP 15B
32	1		1.0													..
48	1		1.0													..
64	1		1.0													..
80	1		1.0													..
96	1		1.0													..
112	1		1.0													..
128	1		1.0													..
144	1		1.0													..
160	1		1.0													..
176	1		1.0													..
192	1		1.0													..
208	1		1.0													..
224	1		1.0													..
240	1		1.0													..
256	1		1.0													..
16	1	6														..
	0.0		1.0		2.0		3.0		4.0		50.0					GROUP 16-IIA
	0.0		12.5		10.0		0.0		0.0		0.0					B
	0.0		12.5		10.0		0.0		0.0		0.0					C
32	1	6														D
	0.0		1.0		2.0		3.0		4.0		50.0					GROUP 16-IIA
	0.0		25.0		20.0		0.0		0.0		0.0					B
	0.0		25.0		20.0		0.0		0.0		0.0					C
48	1	6														D
	0.0		1.0		2.0		3.0		4.0		50.0					GROUP 16-IIA
	0.0		25.0		20.0		0.0		0.0		0.0					B
	0.0		25.0		20.0		0.0		0.0		0.0					C
64	1	6														D
	0.0		1.0		2.0		3.0		4.0		50.0					GROUP 16-IIA
	0.0		25.0		20.0		0.0		0.0		0.0					B
	0.0		25.0		20.0		0.0		0.0		0.0					C
80	1	6														D
	0.0		1.0		2.0		3.0		4.0		50.0					GROUP 16-IIA
	0.0		25.0		20.0		0.0		0.0		0.0					B
																C

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Table 10.4. Output for the Two-Dimensional Solute Transport Problem.

```

*****
                        THIS OUTPUT GENERATED BY VAM2D v. 5.2
                        INPUT FILE NAME = a:tbl10.3
*****

NUMBER OF PROBLEMS TO BE SOLVED = 1

PROBLEM NUMBER: 1

PROBLEM TITLE
-----

TEST PROBLEM 2      (TRANSPORT ONLY)
-----

PROBLEM SPECIFICATION PARAMETERS
-----
MODEL OPTION PARAMETER .....(IMODL) = 0
  NOTE: IMODL = 0 FOR SOLUTE TRANSPORT ONLY
           = 1 FOR WATER FLOW ONLY
           = 2 FOR COUPLED FLOW AND TRANSPORT
HYSTERETIC SOIL MOISTURE (1=YES, 0=NO)....(IHYST) = 0
ANISOTROPIC REL. COND.(1=YES, 0=NO).....(IANI) = 0
CONVERT INITIAL HEAD VALUES(1=YES, 0=NO).(INTSPC) = 0
CHAIN-DECAY REACTIONS(1=YES, 0=NO).....(ICHAIN) = 0
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) = 256
TOTAL NUMBER OF ELEMENTS .....(NE) = 225
SEQUENTIAL NUMBERING INDEX (0=Y, 1=X-DIR) (ISWAP) = 0
AXISYMMETRIC SIMULATION(1=YES, 0=NO).....(IAXSYM) = 0
NUMBER OF POROUS MATRIX MATERIALS .....(NMAT) = 3
INITIAL CONDITION NON-UNIFORMITY INDEX.....(NONU) = 0
NUMBER OF INFIL./EVAP. ELEMENTS .....(NEIEVP) = 0
NUMBER PLANT SPECIES .....(NPLANT) = 0

TIME STEPPING AND ITERATION CONTROL PARAMETERS
-----
TIME STEPPING INDEX (0=CNTRL, 1=BCKWD) ...(IKALL) = 1
TYPE OF ITERATION SCHEME (1=NEWT,0=PICARD)(INEWT) = 0
MAXIMUM NON-LINEAR ITERATIONS .....(NITMAX) = 1
MAXIMUM NUMBER OF TIME STEP REFINEMENTS ..(IRESOL) = 0
LUMPING OF ELEMENT MATRIX (1=YES, 0=NO) ..(ILUMP) = 0

INPUT / OUTPUT CONTROL PARAMETERS
-----
VELOCITY/SATURATION INPUT.....(NVREAD) = 2
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 DATA, 3=NO MESH AND I.C. DATA.....(IPRD) = 2
UNIT 9 OUTPUT OF VEL / SAT (1=YES, 0=NO).(NVWRIT) = 0
VELOCITY PRINTOUT CONTROL INDEX.....(NVPR) = 5
UNIT 10 OUTPUT HEAD/CONC. (0=NONE, N=NTH).(NPLT) = 5

```


NODAL VALUE PRINTOUT CONTROL INDEX.....(NSTEP) = 5
 OBSERVATION NODE INDEX.....(IOBSND) = 1
 MASS BALANCE TO BE PERFORMED (1=YES,0=NO).(IMBAL) = 1
 UNIT 8 OUTPUT OF HEAD/CONC (1=YES, 0=NO).(NOWRIT) = 0
 PRINT CHECK OPTION INDEX.....(IPRCHK) = 0

TEMPORAL DISCRETIZATION DATA

 INITIAL TIME VALUE (TIMA) = 0.0000E+00
 VALUE OF FIRST TIME STEP (TIN) = 0.5000E+00
 TIME STEP MULTIPLIER (TFAC) = 0.1000E+01
 MAXIMUM TIME STEP SIZE (TMAX) = 0.1000E+01

*** LIST OF GENERATED TIME VALUES ***

 0.500E+00 0.100E+01 0.150E+01 0.200E+01 0.250E+01

DEFAULT INITIAL CONCENTRATION VALUE

 0.0000E+00

ELEMENT PROPERTY NUMBERS

1	1	1	1	1	1	1	2	2	2	2	2	2	3	3	1
1	1	1	1	1	1	2	2	2	2	2	2	3	3	1	1
1	1	1	1	1	2	2	2	2	2	2	3	3	1	1	1
1	1	1	1	2	2	2	2	2	2	3	3	1	1	1	1
1	1	2	2	2	2	2	2	3	3	1	1	1	1	1	1
1	2	2	2	2	2	2	3	3	1	1	1	1	1	1	1
2	2	2	2	2	2	3	3	1	1	1	1	1	1	1	2
2	2	2	2	2	3	3	1	1	1	1	1	1	1	2	2
2	2	2	3	3	1	1	1	1	1	1	1	2	2	2	2
2	2	3	3	1	1	1	1	1	1	1	2	2	2	2	2
2	3	3	1	1	1	1	1	1	1	2	2	2	2	2	2
3	3	1	1	1	1	1	1	1	2	2	2	2	2	2	3

TRANSPORT PROPERTIES OF POROUS MEDIA

 MATERIAL NUMBER: 1 (I)

LONGITUDINAL DISPERSIVITY ALPHA-L(PROPJ(I,1)) = 0.2000E+01
 TRANSVERSE DISPERSIVITY ALPHA-T(PROPJ(I,2)) = 0.2000E+01
 MOLECULAR DIFFUSION COMPONENT D-XX....(PROPJ(I,3)) = 0.0000E+00
 MOLECULAR DIFFUSION COMPONENT D-YY....(PROPJ(I,4)) = 0.0000E+00
 EFFECTIVE POROSITY(0 FOR STEADY STATE)(PROPJ(I,5)) = 0.4100E+00
 BULK DENSITY (g/cm**2)(PROPJ(I,6)) = 0.1650E+01

MATERIAL NUMBER: 2 (I)

LONGITUDINAL DISPERSIVITY ALPHA-L(PROPJ(I,1)) = 0.2000E+01
 TRANSVERSE DISPERSIVITY ALPHA-T(PROPJ(I,2)) = 0.2000E+01
 MOLECULAR DIFFUSION COMPONENT D-XX....(PROPJ(I,3)) = 0.0000E+00
 MOLECULAR DIFFUSION COMPONENT D-YY....(PROPJ(I,4)) = 0.0000E+00
 EFFECTIVE POROSITY(0 FOR STEADY STATE)(PROPJ(I,5)) = 0.4300E+00
 BULK DENSITY (g/cm**2)(PROPJ(I,6)) = 0.1550E+01

MATERIAL NUMBER: 3 (I)

LONGITUDINAL DISPERSIVITY ALPHA-L(PROPJ(I,1)) = 0.2000E+01
 TRANSVERSE DISPERSIVITY ALPHA-T(PROPJ(I,2)) = 0.2000E+01
 MOLECULAR DIFFUSION COMPONENT D-XX....(PROPJ(I,3)) = 0.0000E+00

MOLECULAR DIFFUSION COMPONENT D-YY....(PROPJ(I,4)) = 0.0000E+00
EFFECTIVE POROSITY(0 FOR STEADY STATE)(PROPJ(I,5)) = 0.4500E+00
BULK DENSITY (g/cm**2)(PROPJ(I,6)) = 0.1500E+01

SOLUTE PROPERTIES

MATERIAL NUMBER: 1 (I)
DECAY COEFFICIENT (RPROP(I,1)) = 0.0000E+00
DISTRIBUTION COEFFICIENT (cm**3/g)... (RPROP(I,2)) = 0.0000E+00

MATERIAL NUMBER: 2 (I)
DECAY COEFFICIENT (RPROP(I,1)) = 0.0000E+00
DISTRIBUTION COEFFICIENT (cm**3/g)... (RPROP(I,2)) = 0.0000E+00

MATERIAL NUMBER: 3 (I)
DECAY COEFFICIENT (RPROP(I,1)) = 0.0000E+00
DISTRIBUTION COEFFICIENT (cm**3/g)... (RPROP(I,2)) = 0.0000E+00

X-COORDINATES OF GRID LINES

0.00	2.50	5.00	7.50	10.00	12.50	15.00	17.50
20.00	22.50	25.00	30.00	35.00	40.00	45.00	50.00

Y-COORDINATES OF GRID LINES

0.00	10.00	20.00	30.00	40.00	50.00	55.00	60.00
65.00	70.00	75.00	80.00	85.00	90.00	95.00	100.00

BOUNDARY CONDITION DATA

NUMBER OF STEADY DIRICHLET NODES (NBTO) = 16
NUMBER OF STEADY FLUX NODES (NDFLUX) = 0
NUMBER OF TRANSIENT DIRICHLET NODES (NBHVAR) = 0
NUMBER OF TRANSIENT FLUX NODES (NBFVAR) = 16

DIRICHLET BOUNDARY CONDITION DATA

INDEX	NODE NUMBER	DEP. VAR. #	PRESCRIBED VALUE
1	16	1	1.000
2	32	1	1.000
3	48	1	1.000
4	64	1	1.000
5	80	1	1.000
6	96	1	1.000
7	112	1	1.000
8	128	1	1.000
9	144	1	1.000
10	160	1	1.000
11	176	1	1.000
12	192	1	1.000
13	208	1	1.000
14	224	1	1.000
15	240	1	1.000
16	256	1	1.000

TIME DEPENDENT FLUX B. C. FOR
NODE # 16 DEPENDENT VARIABLE # 1

NUMBER OF CONTROL POINTS IN THE TIME GRAPH = 6
 TEMPORAL VARIATION (0=CONTINUOUS, 1=STEP) = 0

TIME VERSUS PRESCRIBED SOLUTE MASS AND WATER AND WATER VOLUMETRIC FLUXES

0.0000E+00	0.0000E+00	0.0000E+00	1.000	12.50	12.50
2.000	10.00	10.00	3.000	0.0000E+00	0.0000E+00
4.000	0.0000E+00	0.0000E+00	50.00	0.0000E+00	0.0000E+00

TIME DEPENDENT FLUX B. C. FOR
 NODE # 32 DEPENDENT VARIABLE # 1

NUMBER OF CONTROL POINTS IN THE TIME GRAPH = 6
 TEMPORAL VARIATION (0=CONTINUOUS, 1=STEP) = 0

TIME VERSUS PRESCRIBED SOLUTE MASS AND WATER AND WATER VOLUMETRIC FLUXES

0.0000E+00	0.0000E+00	0.0000E+00	1.000	25.00	25.00
2.000	20.00	20.00	3.000	0.0000E+00	0.0000E+00
4.000	0.0000E+00	0.0000E+00	50.00	0.0000E+00	0.0000E+00

TIME DEPENDENT FLUX B. C. FOR
 NODE # 48 DEPENDENT VARIABLE # 1

NUMBER OF CONTROL POINTS IN THE TIME GRAPH = 6
 TEMPORAL VARIATION (0=CONTINUOUS, 1=STEP) = 0

TIME VERSUS PRESCRIBED SOLUTE MASS AND WATER AND WATER VOLUMETRIC FLUXES

0.0000E+00	0.0000E+00	0.0000E+00	1.000	25.00	25.00
2.000	20.00	20.00	3.000	0.0000E+00	0.0000E+00
4.000	0.0000E+00	0.0000E+00	50.00	0.0000E+00	0.0000E+00

TIME DEPENDENT FLUX B. C. FOR
 NODE # 64 DEPENDENT VARIABLE # 1

NUMBER OF CONTROL POINTS IN THE TIME GRAPH = 6
 TEMPORAL VARIATION (0=CONTINUOUS, 1=STEP) = 0

TIME VERSUS PRESCRIBED SOLUTE MASS AND WATER AND WATER VOLUMETRIC FLUXES

0.0000E+00	0.0000E+00	0.0000E+00	1.000	25.00	25.00
2.000	20.00	20.00	3.000	0.0000E+00	0.0000E+00
4.000	0.0000E+00	0.0000E+00	50.00	0.0000E+00	0.0000E+00

TIME DEPENDENT FLUX B. C. FOR
 NODE # 80 DEPENDENT VARIABLE # 1

NUMBER OF CONTROL POINTS IN THE TIME GRAPH = 6
 TEMPORAL VARIATION (0=CONTINUOUS, 1=STEP) = 0

TIME VERSUS PRESCRIBED SOLUTE MASS AND WATER AND WATER VOLUMETRIC FLUXES

0.0000E+00	0.0000E+00	0.0000E+00	1.000	25.00	25.00
2.000	20.00	20.00	3.000	0.0000E+00	0.0000E+00
4.000	0.0000E+00	0.0000E+00	50.00	0.0000E+00	0.0000E+00

TIME DEPENDENT FLUX B. C. FOR
 NODE # 96 DEPENDENT VARIABLE # 1

NUMBER OF CONTROL POINTS IN THE TIME GRAPH = 6
 TEMPORAL VARIATION (0=CONTINUOUS, 1=STEP) = 0

TIME VERSUS PRESCRIBED SOLUTE MASS AND WATER AND WATER VOLUMETRIC FLUXES

0.0000E+00	0.0000E+00	0.0000E+00	1.000	25.00	25.00
2.000	20.00	20.00	3.000	0.0000E+00	0.0000E+00
4.000	0.0000E+00	0.0000E+00	50.00	0.0000E+00	0.0000E+00

TIME DEPENDENT FLUX B. C. FOR
 NODE # 112 DEPENDENT VARIABLE # 1

NUMBER OF CONTROL POINTS IN THE TIME GRAPH = 6
 TEMPORAL VARIATION (0=CONTINUOUS, 1=STEP) = 0

TIME VERSUS PRESCRIBED SOLUTE MASS AND WATER AND WATER VOLUMETRIC FLUXES

0.0000E+00	0.0000E+00	0.0000E+00	1.000	25.00	25.00
2.000	20.00	20.00	3.000	0.0000E+00	0.0000E+00
4.000	0.0000E+00	0.0000E+00	50.00	0.0000E+00	0.0000E+00

TIME DEPENDENT FLUX B. C. FOR
 NODE # 128 DEPENDENT VARIABLE # 1

NUMBER OF CONTROL POINTS IN THE TIME GRAPH = 6
 TEMPORAL VARIATION (0=CONTINUOUS, 1=STEP) = 0

TIME VERSUS PRESCRIBED SOLUTE MASS AND WATER AND WATER VOLUMETRIC FLUXES

0.0000E+00	0.0000E+00	0.0000E+00	1.000	25.00	25.00
2.000	20.00	20.00	3.000	0.0000E+00	0.0000E+00
4.000	0.0000E+00	0.0000E+00	50.00	0.0000E+00	0.0000E+00

TIME DEPENDENT FLUX B. C. FOR
 NODE # 144 DEPENDENT VARIABLE # 1

NUMBER OF CONTROL POINTS IN THE TIME GRAPH = 6
 TEMPORAL VARIATION (0=CONTINUOUS, 1=STEP) = 0

TIME VERSUS PRESCRIBED SOLUTE MASS AND WATER AND WATER VOLUMETRIC FLUXES

0.0000E+00	0.0000E+00	0.0000E+00	1.000	25.00	25.00
2.000	20.00	20.00	3.000	0.0000E+00	0.0000E+00
4.000	0.0000E+00	0.0000E+00	50.00	0.0000E+00	0.0000E+00

TIME DEPENDENT FLUX B. C. FOR
 NODE # 160 DEPENDENT VARIABLE # 1

NUMBER OF CONTROL POINTS IN THE TIME GRAPH = 6
 TEMPORAL VARIATION (0=CONTINUOUS, 1=STEP) = 0

TIME VERSUS PRESCRIBED SOLUTE MASS AND WATER AND WATER VOLUMETRIC FLUXES

0.0000E+00	0.0000E+00	0.0000E+00	1.000	25.00	25.00
2.000	20.00	20.00	3.000	0.0000E+00	0.0000E+00
4.000	0.0000E+00	0.0000E+00	50.00	0.0000E+00	0.0000E+00

TIME DEPENDENT FLUX B. C. FOR
 NODE # 176 DEPENDENT VARIABLE # 1

NUMBER OF CONTROL POINTS IN THE TIME GRAPH = 6
 TEMPORAL VARIATION (0=CONTINUOUS, 1=STEP) = 0

TIME VERSUS PRESCRIBED SOLUTE MASS AND WATER AND WATER VOLUMETRIC FLUXES

0.0000E+00	0.0000E+00	0.0000E+00	1.000	37.50	37.50
2.000	30.00	30.00	3.000	0.0000E+00	0.0000E+00
4.000	0.0000E+00	0.0000E+00	50.00	0.0000E+00	0.0000E+00

TIME DEPENDENT FLUX B. C. FOR
 NODE # 192 DEPENDENT VARIABLE # 1

NUMBER OF CONTROL POINTS IN THE TIME GRAPH = 6
 TEMPORAL VARIATION (0=CONTINUOUS, 1=STEP) = 0

TIME VERSUS PRESCRIBED SOLUTE MASS AND WATER AND WATER VOLUMETRIC FLUXES

0.0000E+00	0.0000E+00	0.0000E+00	1.000	50.00	50.00
2.000	40.00	40.00	3.000	0.0000E+00	0.0000E+00
4.000	0.0000E+00	0.0000E+00	50.00	0.0000E+00	0.0000E+00

TIME DEPENDENT FLUX B. C. FOR
 NODE # 208 DEPENDENT VARIABLE # 1

NUMBER OF CONTROL POINTS IN THE TIME GRAPH = 6
 TEMPORAL VARIATION (0=CONTINUOUS, 1=STEP) = 0

TIME VERSUS PRESCRIBED SOLUTE MASS AND WATER AND WATER VOLUMETRIC FLUXES

0.0000E+00	0.0000E+00	0.0000E+00	1.000	50.00	50.00
2.000	40.00	40.00	3.000	0.0000E+00	0.0000E+00
4.000	0.0000E+00	0.0000E+00	50.00	0.0000E+00	0.0000E+00

TIME DEPENDENT FLUX B. C. FOR
 NODE # 224 DEPENDENT VARIABLE # 1

NUMBER OF CONTROL POINTS IN THE TIME GRAPH = 6
 TEMPORAL VARIATION (0=CONTINUOUS, 1=STEP) = 0

TIME VERSUS PRESCRIBED SOLUTE MASS AND WATER AND WATER VOLUMETRIC FLUXES

0.0000E+00	0.0000E+00	0.0000E+00	1.000	50.00	50.00
2.000	40.00	40.00	3.000	0.0000E+00	0.0000E+00
4.000	0.0000E+00	0.0000E+00	50.00	0.0000E+00	0.0000E+00

TIME DEPENDENT FLUX B. C. FOR
 NODE # 240 DEPENDENT VARIABLE # 1

NUMBER OF CONTROL POINTS IN THE TIME GRAPH = 6
 TEMPORAL VARIATION (0=CONTINUOUS, 1=STEP) = 0

TIME VERSUS PRESCRIBED SOLUTE MASS AND WATER AND WATER VOLUMETRIC FLUXES

0.0000E+00	0.0000E+00	0.0000E+00	1.000	50.00	50.00
2.000	40.00	40.00	3.000	0.0000E+00	0.0000E+00

4.000 0.0000E+00 0.0000E+00 50.00 0.0000E+00 0.0000E+00

TIME DEPENDENT FLUX B. C. FOR
NODE # 256 DEPENDENT VARIABLE # 1

NUMBER OF CONTROL POINTS IN THE TIME GRAPH = 6
TEMPORAL VARIATION (0=CONTINUOUS, 1=STEP) = 0

TIME VERSUS PRESCRIBED SOLUTE MASS AND WATER AND WATER VOLUMETRIC FLUXES

0.0000E+00	0.0000E+00	0.0000E+00	1.000	25.00	25.00
2.000	20.00	20.00	3.000	0.0000E+00	0.0000E+00
4.000	0.0000E+00	0.0000E+00	50.00	0.0000E+00	0.0000E+00

DEFAULT VALUES AND WEIGHTING FACTORS

DEFAULT VALUE OF X-VELOCITY(VCX) = 0.0000E+00
DEFAULT VALUE OF Y-VELOCITY(VCY) = 0.0000E+00
X-DIRECTION UPSTREAM WEIGHTING FACTOR(WFAC) = 0.0000E+00
Y-DIRECTION UPSTREAM WEIGHTING FACTOR(YFAC) = 0.0000E+00
DEFAULT WATER SATURATION(SWD) = 0.0000E+00
STEADY-STATE VELOCITY FIELD (0=NO, 1=YES).(IVSTED) = 0

LIST OF BOUNDARY NODE NUMBERS:

1 16 17 32 33 48 49 64 65 80 81 96 97 112 113 128
129 144 145 160 161 176 177 192 193 208 209 224 225 240 241 256

----- ACTUAL HALF BAND WIDTH = 17 FULL BANDWIDTH = 35 -----

LIST OF OBSERVATION NODES

62 126 150 174 222

+++++++ BEGIN TRANSIENT CALCULATIONS +++++++

**** ELAPSED SIMULATION TIME : 0.5000 TIME STEP NUMBER : 1 TIME STEP SIZE: 0.500E+00 ****

**** ELAPSED SIMULATION TIME : 1.000 TIME STEP NUMBER : 2 TIME STEP SIZE: 0.500E+00 ****

**** ELAPSED SIMULATION TIME : 1.500 TIME STEP NUMBER : 3 TIME STEP SIZE: 0.500E+00 ****

**** ELAPSED SIMULATION TIME : 2.000 TIME STEP NUMBER : 4 TIME STEP SIZE: 0.500E+00 ****

**** ELAPSED SIMULATION TIME : 2.500 TIME STEP NUMBER : 5 TIME STEP SIZE: 0.500E+00 ****

*** ELEMENTAL FLUID VELOCITY FROM TAPE 9 ***

ELEMENT	X-VELOCITY	Y-VELOCITY	ELEMENT	X-VELOCITY	Y-VELOCITY	ELEMENT	X-VELOCITY	Y-VELOCITY
1	0.000E+00	-5.11	2	0.000E+00	-5.10	3	6.633E-14	-5.09
4	6.246E-14	-5.07	5	0.000E+00	-5.04	6	0.000E+00	-5.02
7	0.000E+00	-5.01	8	5.705E-14	-4.95	9	1.130E-13	-4.85
10	5.596E-14	-4.75	11	0.000E+00	-4.63	12	0.000E+00	-4.51
13	0.000E+00	-4.38	14	3.702E-14	-4.25	15	3.687E-14	-4.09
16	-7.622E-14	-5.11	17	-7.085E-14	-5.10	18	1.327E-13	-5.09
19	1.249E-13	-5.07	20	-5.913E-14	-5.04	21	-1.138E-13	-5.02
22	-1.111E-13	-5.01	23	-5.705E-14	-4.95	24	0.000E+00	-4.85
25	5.596E-14	-4.75	26	5.543E-14	-4.63	27	-5.490E-14	-4.51
28	5.438E-14	-4.38	29	1.111E-13	-4.25	30	1.106E-13	-4.09
31	0.000E+00	-5.11	32	2.126E-13	-5.10	33	2.653E-13	-5.09
34	1.249E-13	-5.07	35	5.913E-14	-5.04	36	0.000E+00	-5.02
37	0.000E+00	-5.01	38	-1.141E-13	-4.95	39	-1.130E-13	-4.85
40	5.596E-14	-4.75	41	0.000E+00	-4.63	42	0.000E+00	-4.51
43	5.438E-14	-4.38	44	3.702E-14	-4.25	45	0.000E+00	-4.09
46	7.622E-14	-5.11	47	1.417E-13	-5.10	48	1.327E-13	-5.09
49	2.498E-13	-5.07	50	5.913E-14	-5.04	51	-1.138E-13	-5.02
52	-1.666E-13	-5.01	53	-1.712E-13	-4.95	54	-5.650E-14	-4.85
55	-1.119E-13	-4.75	56	-5.543E-14	-4.63	57	5.490E-14	-4.51
58	1.631E-13	-4.38	59	1.851E-13	-4.25	60	1.475E-13	-4.09
61	1.524E-13	-5.11	62	2.126E-13	-5.10	63	1.327E-13	-5.09
64	1.249E-13	-5.07	65	5.913E-14	-5.04	66	-5.688E-14	-5.02
67	-2.221E-13	-5.01	68	-1.712E-13	-4.95	69	-2.260E-13	-4.85
70	-1.119E-13	-4.75	71	1.109E-13	-4.63	72	1.098E-13	-4.51
73	1.631E-13	-4.38	74	1.111E-13	-4.25	75	1.475E-13	-4.09
76	2.287E-13	-5.11	77	3.543E-13	-5.10	78	2.653E-13	-5.09
79	1.249E-13	-5.07	80	1.183E-13	-5.04	81	0.000E+00	-5.02
82	-1.666E-13	-5.01	83	-1.712E-13	-4.95	84	-5.650E-14	-4.85
85	0.000E+00	-4.75	86	5.543E-14	-4.63	87	1.647E-13	-4.51
88	1.088E-13	-4.38	89	7.403E-14	-4.25	90	1.106E-13	-4.09
91	2.287E-13	-5.11	92	3.543E-13	-5.10	93	2.653E-13	-5.09
94	1.249E-13	-5.07	95	1.183E-13	-5.04	96	1.138E-13	-5.02
97	0.000E+00	-5.01	98	-2.282E-13	-4.95	99	-1.695E-13	-4.85
100	5.596E-14	-4.75	101	1.109E-13	-4.63	102	0.000E+00	-4.51
103	-1.088E-13	-4.38	104	1.111E-13	-4.25	105	2.212E-13	-4.09
106	1.524E-13	-5.11	107	2.834E-13	-5.10	108	1.327E-13	-5.09

109	0.000E+00	-5.07	110	1.183E-13	-5.04	111	2.275E-13	-5.02
112	5.553E-14	-5.01	113	-5.705E-14	-4.95	114	0.000E+00	-4.85
115	0.000E+00	-4.75	116	0.000E+00	-4.63	117	0.000E+00	-4.51
118	0.000E+00	-4.38	119	-3.702E-14	-4.25	120	3.687E-14	-4.09
121	0.000E+00	-5.11	122	2.126E-13	-5.10	123	2.653E-13	-5.09
124	1.249E-13	-5.07	125	1.183E-13	-5.04	126	1.706E-13	-5.02
127	5.553E-14	-5.01	128	-5.705E-14	-4.95	129	-1.130E-13	-4.85
130	-1.679E-13	-4.75	131	-1.663E-13	-4.63	132	-1.098E-13	-4.51
133	-5.438E-14	-4.38	134	7.403E-14	-4.25	135	7.374E-14	-4.09
136	0.000E+00	-5.11	137	1.417E-13	-5.10	138	2.653E-13	-5.09
139	1.249E-13	-5.07	140	0.000E+00	-5.04	141	5.688E-14	-5.02
142	1.111E-13	-5.01	143	1.141E-13	-4.95	144	-5.650E-14	-4.85
145	-1.679E-13	-4.75	146	-1.109E-13	-4.63	147	-5.490E-14	-4.51
148	0.000E+00	-4.38	149	3.702E-14	-4.25	150	0.000E+00	-4.09
151	3.811E-14	-5.11	152	1.063E-13	-5.10	153	1.990E-13	-5.09
154	9.369E-14	-5.07	155	-5.913E-14	-5.04	156	-2.844E-14	-5.02
157	1.388E-13	-5.01	158	1.426E-13	-4.95	159	0.000E+00	-4.85
160	-1.679E-13	-4.75	161	-1.386E-13	-4.63	162	8.235E-14	-4.51
163	8.156E-14	-4.38	164	-1.851E-14	-4.25	165	-7.374E-14	-4.09
166	-3.811E-14	-5.11	167	3.543E-14	-5.10	168	6.633E-14	-5.09
169	3.123E-14	-5.07	170	2.956E-14	-5.04	171	0.000E+00	-5.02
172	-2.776E-14	-5.01	173	-5.705E-14	-4.95	174	-1.130E-13	-4.85
175	-2.798E-14	-4.75	176	0.000E+00	-4.63	177	-1.098E-13	-4.51
178	-1.359E-13	-4.38	179	-5.553E-14	-4.25	180	0.000E+00	-4.09
181	7.622E-14	-5.11	182	7.085E-14	-5.10	183	3.316E-14	-5.09
184	3.123E-14	-5.07	185	2.956E-14	-5.04	186	0.000E+00	-5.02
187	-5.553E-14	-5.01	188	-1.997E-13	-4.95	189	-2.260E-13	-4.85
190	-1.959E-13	-4.75	191	-1.386E-13	-4.63	192	-1.098E-13	-4.51
193	-5.438E-14	-4.38	194	0.000E+00	-4.25	195	0.000E+00	-4.09
196	0.000E+00	-5.11	197	0.000E+00	-5.10	198	3.316E-14	-5.09
199	3.123E-14	-5.07	200	-2.956E-14	-5.04	201	-5.688E-14	-5.02
202	-8.329E-14	-5.01	203	-5.705E-14	-4.95	204	-2.825E-14	-4.85
205	-5.596E-14	-4.75	206	-8.314E-14	-4.63	207	-2.745E-14	-4.51
208	-2.719E-14	-4.38	209	-1.851E-14	-4.25	210	0.000E+00	-4.09
211	0.000E+00	-5.11	212	0.000E+00	-5.10	213	0.000E+00	-5.09
214	3.123E-14	-5.07	215	-2.956E-14	-5.04	216	-8.532E-14	-5.02
217	-2.776E-14	-5.01	218	5.705E-14	-4.95	219	5.650E-14	-4.85
220	2.798E-14	-4.75	221	5.543E-14	-4.63	222	0.000E+00	-4.51
223	-8.156E-14	-4.38	224	-7.403E-14	-4.25	225	-3.687E-14	-4.09

ELEMENT SATURATION VALUES FROM TAPE 9

ELEMENT	SAT. VALUE	ELEMENT	SAT. VALUE	ELEMENT	SAT. VALUE	ELEMENT	SAT. VALUE	ELEMENT	SAT. VALUE
1	9.3511E-02	2	9.0968E-02	3	8.8824E-02	4	8.6994E-02	5	8.5415E-02
6	8.4350E-02	7	8.3709E-02	8	0.4478	9	0.4442	10	0.4407
11	0.4373	12	0.4338	13	0.4304	14	0.6298	15	0.6275
16	9.3511E-02	17	9.0968E-02	18	8.8824E-02	19	8.6994E-02	20	8.5415E-02
21	8.4350E-02	22	8.3709E-02	23	0.4478	24	0.4442	25	0.4407
26	0.4373	27	0.4338	28	0.4304	29	0.6298	30	0.6275
31	9.3511E-02	32	9.0968E-02	33	8.8824E-02	34	8.6994E-02	35	8.5415E-02
36	8.4350E-02	37	8.3709E-02	38	0.4478	39	0.4442	40	0.4407
41	0.4373	42	0.4338	43	0.4304	44	0.6298	45	0.6275
46	9.3511E-02	47	9.0968E-02	48	8.8824E-02	49	8.6994E-02	50	8.5415E-02
51	8.4350E-02	52	8.3709E-02	53	0.4478	54	0.4442	55	0.4407
56	0.4373	57	0.4338	58	0.4304	59	0.6298	60	0.6275
61	9.3511E-02	62	9.0968E-02	63	8.8824E-02	64	8.6994E-02	65	8.5415E-02
66	8.4350E-02	67	8.3709E-02	68	0.4478	69	0.4442	70	0.4407
71	0.4373	72	0.4338	73	0.4304	74	0.6298	75	0.6275
76	9.3511E-02	77	9.0968E-02	78	8.8824E-02	79	8.6994E-02	80	8.5415E-02
81	8.4350E-02	82	8.3709E-02	83	0.4478	84	0.4442	85	0.4407
86	0.4373	87	0.4338	88	0.4304	89	0.6298	90	0.6275
91	9.3511E-02	92	9.0968E-02	93	8.8824E-02	94	8.6994E-02	95	8.5415E-02
96	8.4350E-02	97	8.3709E-02	98	0.4478	99	0.4442	100	0.4407
101	0.4373	102	0.4338	103	0.4304	104	0.6298	105	0.6275
106	9.3511E-02	107	9.0968E-02	108	8.8824E-02	109	8.6994E-02	110	8.5415E-02
111	8.4350E-02	112	8.3709E-02	113	0.4478	114	0.4442	115	0.4407
116	0.4373	117	0.4338	118	0.4304	119	0.6298	120	0.6275
121	9.3511E-02	122	9.0968E-02	123	8.8824E-02	124	8.6994E-02	125	8.5415E-02
126	8.4350E-02	127	8.3709E-02	128	0.4478	129	0.4442	130	0.4407

131	0.4373	132	0.4338	133	0.4304	134	0.6298	135	0.6275
136	9.3511E-02	137	9.0968E-02	138	8.8824E-02	139	8.6994E-02	140	8.5415E-02
141	8.4350E-02	142	8.3709E-02	143	0.4478	144	0.4442	145	0.4407
146	0.4373	147	0.4338	148	0.4304	149	0.6298	150	0.6275
151	9.3511E-02	152	9.0968E-02	153	8.8824E-02	154	8.6994E-02	155	8.5415E-02
156	8.4350E-02	157	8.3709E-02	158	0.4478	159	0.4442	160	0.4407
161	0.4373	162	0.4338	163	0.4304	164	0.6298	165	0.6275
166	9.3511E-02	167	9.0968E-02	168	8.8824E-02	169	8.6994E-02	170	8.5415E-02
171	8.4350E-02	172	8.3709E-02	173	0.4478	174	0.4442	175	0.4407
176	0.4373	177	0.4338	178	0.4304	179	0.6298	180	0.6275
181	9.3511E-02	182	9.0968E-02	183	8.8824E-02	184	8.6994E-02	185	8.5415E-02
186	8.4350E-02	187	8.3709E-02	188	0.4478	189	0.4442	190	0.4407
191	0.4373	192	0.4338	193	0.4304	194	0.6298	195	0.6275
196	9.3511E-02	197	9.0968E-02	198	8.8824E-02	199	8.6994E-02	200	8.5415E-02
201	8.4350E-02	202	8.3709E-02	203	0.4478	204	0.4442	205	0.4407
206	0.4373	207	0.4338	208	0.4304	209	0.6298	210	0.6275
211	9.3511E-02	212	9.0968E-02	213	8.8824E-02	214	8.6994E-02	215	8.5415E-02
216	8.4350E-02	217	8.3709E-02	218	0.4478	219	0.4442	220	0.4407
221	0.4373	222	0.4338	223	0.4304	224	0.6298	225	0.6275

*** NODAL DISPERSIVE FLUX VALUES ***

NODE	DISP. FLUX	NODE	DISP. FLUX	NODE	DISP. FLUX	NODE	DISP. FLUX	NODE	DISP. FLUX
1	-1.8319E-15	16	6.8543E-04	17	-4.7740E-15	32	1.3709E-03	33	-1.1102E-16
48	1.3709E-03	49	-3.4417E-15	64	1.3709E-03	65	2.2204E-16	80	1.3709E-03
81	5.5511E-15	96	1.3709E-03	97	-2.2204E-15	112	1.3709E-03	113	-1.7764E-15
128	1.3709E-03	129	3.1086E-15	144	1.3709E-03	145	-7.7716E-16	160	1.3709E-03
161	-5.9952E-15	176	2.0563E-03	177	1.9984E-15	192	2.7417E-03	193	1.0436E-14
208	2.7417E-03	209	-1.7764E-15	224	2.7417E-03	225	6.6613E-16	240	2.7417E-03
241	3.3307E-16	256	1.3709E-03						

SUM OF ABOVE FLUX VALUES = 2.74171E-02

*** INCREMENTAL MASS BALANCE RESULTS OVER A TIME STEP ***

TOTAL DISPERSIVE FLUX RATE	2.74171E-02
TOTAL ADVECTIVE FLUX RATE	-9.5146
TOTAL DISPERSIVE + ADVECTIVE FLUX RATE	-9.4872
RATE OF MASS DECAY AND TRANSFORMATION	0.00000E+00
NET RATE OF MATERIAL ACCUMULATION	-9.5508
MASS BALANCE ERROR	6.35852E-02
NORMALIZED MASS BALANCE ERROR	1.34620E-04
RATE OF MASS ACCUMULATION DUE TO PRESSURE HEAD CHANGE	-53.239

*** CUMULATIVE MASS BALANCE RESULTS ***

CUMULATIVE MATERIAL STORAGE	492.45
CUMULATIVE MASS DECAY AND TRANSFORMATION.....	0.00000E+00

*** NODAL CONCENTRATION VALUES ***

NODE	CONC. VALUE	NODE	CONC. VALUE	NODE	CONC. VALUE	NODE	CONC. VALUE	NODE	CONC. VALUE
1	0.8203	2	0.8311	3	0.8473	4	0.8598	5	0.8726

6	0.8841	7	0.8896	8	0.8950	9	0.9129	10	0.9397
11	0.9601	12	0.9755	13	0.9863	14	0.9931	15	0.9978
16	1.000	17	0.8203	18	0.8311	19	0.8473	20	0.8598
21	0.8726	22	0.8841	23	0.8896	24	0.8950	25	0.9129
26	0.9397	27	0.9601	28	0.9755	29	0.9863	30	0.9931
31	0.9978	32	1.000	33	0.8203	34	0.8311	35	0.8473
36	0.8598	37	0.8726	38	0.8841	39	0.8896	40	0.8950
41	0.9129	42	0.9397	43	0.9601	44	0.9755	45	0.9863
46	0.9931	47	0.9978	48	1.000	49	0.8203	50	0.8311
51	0.8473	52	0.8598	53	0.8726	54	0.8841	55	0.8896
56	0.8950	57	0.9129	58	0.9397	59	0.9601	60	0.9755
61	0.9863	62	0.9931	63	0.9978	64	1.000	65	0.8203
66	0.8311	67	0.8473	68	0.8598	69	0.8726	70	0.8841
71	0.8896	72	0.8950	73	0.9129	74	0.9397	75	0.9601
76	0.9755	77	0.9863	78	0.9931	79	0.9978	80	1.000
81	0.8203	82	0.8311	83	0.8473	84	0.8598	85	0.8726
86	0.8841	87	0.8896	88	0.8950	89	0.9129	90	0.9397
91	0.9601	92	0.9755	93	0.9863	94	0.9931	95	0.9978
96	1.000	97	0.8203	98	0.8311	99	0.8473	100	0.8598
101	0.8726	102	0.8841	103	0.8896	104	0.8950	105	0.9129
106	0.9397	107	0.9601	108	0.9755	109	0.9863	110	0.9931
111	0.9978	112	1.000	113	0.8203	114	0.8311	115	0.8473
116	0.8598	117	0.8726	118	0.8841	119	0.8896	120	0.8950
121	0.9129	122	0.9397	123	0.9601	124	0.9755	125	0.9863
126	0.9931	127	0.9978	128	1.000	129	0.8203	130	0.8311
131	0.8473	132	0.8598	133	0.8726	134	0.8841	135	0.8896
136	0.8950	137	0.9129	138	0.9397	139	0.9601	140	0.9755
141	0.9863	142	0.9931	143	0.9978	144	1.000	145	0.8203
146	0.8311	147	0.8473	148	0.8598	149	0.8726	150	0.8841
151	0.8896	152	0.8950	153	0.9129	154	0.9397	155	0.9601
156	0.9755	157	0.9863	158	0.9931	159	0.9978	160	1.000
161	0.8203	162	0.8311	163	0.8473	164	0.8598	165	0.8726
166	0.8841	167	0.8896	168	0.8950	169	0.9129	170	0.9397
171	0.9601	172	0.9755	173	0.9863	174	0.9931	175	0.9978
176	1.000	177	0.8203	178	0.8311	179	0.8473	180	0.8598
181	0.8726	182	0.8841	183	0.8896	184	0.8950	185	0.9129
186	0.9397	187	0.9601	188	0.9755	189	0.9863	190	0.9931
191	0.9978	192	1.000	193	0.8203	194	0.8311	195	0.8473
196	0.8598	197	0.8726	198	0.8841	199	0.8896	200	0.8950
201	0.9129	202	0.9397	203	0.9601	204	0.9755	205	0.9863
206	0.9931	207	0.9978	208	1.000	209	0.8203	210	0.8311
211	0.8473	212	0.8598	213	0.8726	214	0.8841	215	0.8896
216	0.8950	217	0.9129	218	0.9397	219	0.9601	220	0.9755
221	0.9863	222	0.9931	223	0.9978	224	1.000	225	0.8203
226	0.8311	227	0.8473	228	0.8598	229	0.8726	230	0.8841
231	0.8896	232	0.8950	233	0.9129	234	0.9397	235	0.9601
236	0.9755	237	0.9863	238	0.9931	239	0.9978	240	1.000
241	0.8203	242	0.8311	243	0.8473	244	0.8598	245	0.8726
246	0.8841	247	0.8896	248	0.8950	249	0.9129	250	0.9397
251	0.9601	252	0.9755	253	0.9863	254	0.9931	255	0.9978
256	1.000								

*** OBSERVATION NODE INFORMATION ***

 MODAL VALUES OF DEPENDENT VARIABLE OVER TIME

OBSERVED NODE NUMBER: 62

TIME	CONCENTRATION	TIME	CONCENTRATION	TIME	CONCENTRATION	TIME	CONCENTRATION
----	-----	----	-----	----	-----	----	-----
0.5000E+00	0.4118E+00	0.1000E+01	0.8178E+00	0.1500E+01	0.9469E+00	0.2000E+01	0.9841E+00
0.2500E+01	0.9931E+00						

OBSERVED NODE NUMBER: 126

TIME	CONCENTRATION	TIME	CONCENTRATION	TIME	CONCENTRATION	TIME	CONCENTRATION
----	-----	----	-----	----	-----	----	-----
0.5000E+00	0.4118E+00	0.1000E+01	0.8178E+00	0.1500E+01	0.9469E+00	0.2000E+01	0.9841E+00
0.2500E+01	0.9931E+00						

OBSERVED NODE NUMBER: 150

TIME ----	CONCENTRATION -----	TIME ----	CONCENTRATION -----	TIME ----	CONCENTRATION -----	TIME ----	CONCENTRATION -----
0.5000E+00	0.7407E-01	0.1000E+01	0.3464E+00	0.1500E+01	0.6216E+00	0.2000E+01	0.8038E+00
0.2500E+01	0.8841E+00						

OBSERVED NODE NUMBER: 174

TIME ----	CONCENTRATION -----	TIME ----	CONCENTRATION -----	TIME ----	CONCENTRATION -----	TIME ----	CONCENTRATION -----
0.5000E+00	0.4118E+00	0.1000E+01	0.8178E+00	0.1500E+01	0.9469E+00	0.2000E+01	0.9841E+00
0.2500E+01	0.9931E+00						

OBSERVED NODE NUMBER: 222

TIME ----	CONCENTRATION -----	TIME ----	CONCENTRATION -----	TIME ----	CONCENTRATION -----	TIME ----	CONCENTRATION -----
0.5000E+00	0.4118E+00	0.1000E+01	0.8178E+00	0.1500E+01	0.9469E+00	0.2000E+01	0.9841E+00
0.2500E+01	0.9931E+00						

***** VAM2D HAS FULLY EXECUTED *****

10.4 PROBLEM 3: CONCURRENT SIMULATION OF FLOW AND TRANSPORT

10.4.1 Input Data

The input data file for this sample flow and transport problem is presented in Table 10.5. Note that the modeling parameter option IMODL is now set equal to 2. Also evident in the depicted input data is the specification of NVREAD = 0. The use of IMODL = 2 means that the flow and transport equations will be solved concurrently. Hence there is no need to supply a velocity file. The input data shown in Table 10.5 also contains sixteen prescribed concentration boundary conditions, as well as node numbers of all non-zero flux boundary nodes.

10.4.2 Sample Output

Output of the flow and transport calculation is displayed in Table 10.6. This output consists of the following categories of information:

1. Brief summary of control input data and material hydraulic properties.
2. Prescribed boundary condition data.
3. Initial condition data.
4. Maximum bandwidth of the global matrix for the problem.
5. List of observation nodes.
6. Time-step number.
7. Print check information for the convergence of the nonlinear iterations.
8. Node numbers and nodal head values corresponding to the given time value.
9. List of unsaturated elements and centroidal values of water saturation.
10. List of element numbers and corresponding centroidal values of Darcy velocity components.
11. Fluid mass balance information.

12. Solute mass balance information.
13. Node numbers and concentration values corresponding to the given time value.
14. Observation node information.

Note that information in categories 8-13 is provided only for the 5-th timestep.

Table 10.5. Input Data for the Concurrent Simulation of Unsaturated Flow and Solute Transport Problems.

1	(FLOW AND TRANSPORT SIMULTANEOUSLY)															GROUP 1
TEST PROBLEM 2	0	0	0	0	0	1	5	256	225	0	0	3	0	0	0	GROUP 2
2	0	0	0	0	0	1	5	256	225	0	0	3	0	0	0	GROUP 3
1	0	10	3	1	0.1	5	5	0.0	0	0	0	0	0	0	0	GROUP 4
0	1	0	2	0	5	5	5	1	1	0	0	0	0	0	0	GROUP 5
	0.0		0.5		1.0		1.0									GROUP 6
-100.0			0.0													GROUP 7
1	1	1	1	1	1	1	2	2	2	2	2	2	3	3	1	GROUP 8
1	1	1	1	1	1	1	2	2	2	2	2	2	3	3	1	..
1	1	1	1	1	1	2	2	2	2	2	2	3	3	1	1	..
1	1	1	1	1	2	2	2	2	2	2	3	3	1	1	1	..
1	1	1	1	2	2	2	2	2	3	3	3	1	1	1	1	..
1	1	1	2	2	2	2	2	2	3	3	1	1	1	1	1	..
1	2	2	2	2	2	2	2	3	3	1	1	1	1	1	1	..
2	2	2	2	2	2	2	3	3	1	1	1	1	1	1	2	..
2	2	2	2	2	3	3	1	1	1	1	1	1	1	2	2	..
2	2	2	3	3	1	1	1	1	1	1	1	2	2	2	2	..
2	2	3	3	1	1	1	1	1	1	1	2	2	2	2	2	..
3	3	1	1	1	1	1	1	1	2	2	2	2	2	2	3	..
3																..
0.350E03	0.350E03	0.000E00	0.000E00	0.000E00	0.410E00	0.000E00										GROUP 9
2.500E01	2.500E01	0.000E00	0.000E00	0.000E00	0.430E00	0.000E00										..
1.080E01	1.080E01	0.000E00	0.000E00	0.450E00	0.000E00											GROUP 10
0.0574	1.00	0.124	2.28													..
0.0774	1.00	0.036	1.56													..
0.0675	1.00	0.020	1.41													..
2.0	2.0	0.0	0.0	0.41	1.65											GROUP 11A
2.0	2.0	0.0	0.0	0.43	1.55											..
2.0	2.0	0.0	0.0	0.45	1.50											..
0.0	0.0															GROUP 11B
0.0	0.0															..
0.0	0.0															..
16	16	5.0	10.0	1												GROUP 12
0.0	2.5	5.0	7.5													GROUP 13
20.0	22.5	25.0	30.0													..
0.0	10.0	20.0	30.0													..
65.0	70.0	75.0	80.0													..
32	0	0	16													GROUP 15A
1	1	-100.0														GROUP 15B
17	1	-100.0														..
33	1	-100.0														..
49	1	-100.0														..
65	1	-100.0														..
81	1	-100.0														..
97	1	-100.0														..
113	1	-100.0														..
129	1	-100.0														..
145	1	-100.0														..
161	1	-100.0														..
177	1	-100.0														..
193	1	-100.0														..
209	1	-100.0														..
225	1	-100.0														..
241	1	-100.0														..
16	2	1.0														..
32	2	1.0														..
48	2	1.0														..
64	2	1.0														..
80	2	1.0														..
96	2	1.0														..
112	2	1.0														..
128	2	1.0														..
144	2	1.0														..
160	2	1.0														..
176	2	1.0														..
192	2	1.0														..

Table 10.6. Output for the Concurrent Simulation Run.

```

*****
                        THIS OUTPUT GENERATED BY VAM2D v. 5.2
                        INPUT FILE NAME = a:tbl10.5
*****

NUMBER OF PROBLEMS TO BE SOLVED = 1

PROBLEM NUMBER: 1

PROBLEM TITLE
-----

TEST PROBLEM 2      (FLOW AND TRANSPORT SIMULTANEOUSLY)
-----

PROBLEM SPECIFICATION PARAMETERS
-----
MODEL OPTION PARAMETER .....(IMODL) = 2
NOTE: IMODL = 0 FOR SOLUTE TRANSPORT ONLY
      = 1 FOR WATER FLOW ONLY
      = 2 FOR COUPLED FLOW AND TRANSPORT
HYSTERETIC SOIL MOISTURE (1=YES, 0=NO)....(IHYST) = 0
ANISOTROPIC REL. COND.(1=YES, 0=NO).....(IANI) = 0
CONVERT INITIAL HEAD VALUES(1=YES, 0=NO).(INTSPC) = 0
CHAIN-DECAY REACTIONS(1=YES, 0=NO).....(ICHAIN) = 0
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) = 256
TOTAL NUMBER OF ELEMENTS .....(NE) = 225
SEQUENTIAL NUMBERING INDEX (0=Y, 1=X-DIR) (ISWAP) = 0
AXISYMMETRIC SIMULATION(1=YES, 0=NO)....(IAXSYM) = 0
NUMBER OF POROUS MATRIX MATERIALS .....(NMAT) = 3
INITIAL CONDITION NON-UNIFORMITY INDEX.....(NONU) = 0
NUMBER OF INFIL./EVAP. ELEMENTS .....(NEIEVP) = 0
NUMBER PLANT SPECIES .....(NPLANT) = 0

TIME STEPPING AND ITERATION CONTROL PARAMETERS
-----
TIME STEPPING INDEX (0=CNTRL, 1=BCKWD) ... (IKALL) = 1
TYPE OF ITERATION SCHEME (1=NEWT, 0=PICARD) (INEWT) = 0
MAXIMUM NON-LINEAR ITERATIONS .....(NITMAX) = 10
MAXIMUM NUMBER OF TIME STEP REFINEMENTS ..(IRESOL) = 3
LUMPING OF ELEMENT MATRIX (1=YES, 0=NO) ..(ILUMP) = 1
ABS. ITERATION TOLERANCE FOR HEAD .....(HTOL) = 0.10000E+00
RELATIVE ITERATION TOLERANCE .....(RELCON) = 0.00000E+00
REL. PERMEABILITY UPSTREAM INDEX .....(IUPSTR) = 0
NONLINEAR ITERATION SELECTION .....(ISELSC) = 0

INPUT / OUTPUT CONTROL PARAMETERS
-----
VELOCITY/SATURATION 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 DATA, 3=NO MESH AND I.C. DATA.....(IPRD) =    2
UNIT 9 OUTPUT OF VEL / SAT (1=YES, 0=NO).(NVWRIT) =    0
VELOCITY PRINTOUT CONTROL INDEX.....(NVPR) =    5
UNIT 10 OUTPUT HEAD/CONC. (0=NONE, N=NTH).(NPLT) =    5
NODAL VALUE PRINTOUT CONTROL INDEX.....(NSTP) =    5
OBSERVATION NODE INDEX.....(IOBSND) =    1
MASS BALANCE TO BE PERFORMED (1=YES,0=NO).(IMBAL) =    1
UNIT 8 OUTPUT OF HEAD/CONC (1=YES, 0=NO).(NOWRIT) =    0
PRINT CHECK OPTION INDEX.....(IPRCHK) =    0

```

TEMPORAL DISCRETIZATION DATA

```

-----
INITIAL TIME VALUE ..... (TIMA) = 0.0000E+00
VALUE OF FIRST TIME STEP ..... (TIN) = 0.5000E+00
TIME STEP MULTIPLIER ..... (TFAC) = 0.1000E+01
MAXIMUM TIME STEP SIZE ..... (TMAX) = 0.1000E+01

```

*** LIST OF GENERATED TIME VALUES ***

```

-----
0.500E+00 0.100E+01 0.150E+01 0.200E+01 0.250E+01

```

DEFAULT INITIAL VALUE OF PRESSURE HEAD

```

-----
-0.1000E+03

```

DEFAULT INITIAL CONCENTRATION VALUE

```

-----
0.0000E+00

```

ELEMENT PROPERTY NUMBERS

```

-----
1 1 1 1 1 1 1 2 2 2 2 2 2 3 3 1
1 1 1 1 1 1 2 2 2 2 2 2 3 3 1 1
1 1 1 1 1 2 2 2 2 2 2 3 3 1 1 1
1 1 1 1 2 2 2 2 2 2 3 3 1 1 1 1
1 1 2 2 2 2 2 2 3 3 1 1 1 1 1 1
1 2 2 2 2 2 2 3 3 1 1 1 1 1 1 1
2 2 2 2 2 2 3 3 1 1 1 1 1 1 2
2 2 2 2 2 3 3 1 1 1 1 1 1 1 2 2
2 2 2 2 3 3 1 1 1 1 1 1 1 2 2 2
2 2 3 3 1 1 1 1 1 1 1 2 2 2 2 2
2 3 3 1 1 1 1 1 1 1 2 2 2 2 2 2
3 3 1 1 1 1 1 1 1 2 2 2 2 2 2 3
3

```

HYDRAULIC PROPERTIES OF POROUS MEDIA

```

-----
MATERIAL NUMBER:    1  (1)

```

```

X-DIRECTION HYDRAULIC CONDUCTIVITY ... (PROP(1,1)) = 0.3500E+03
Y-DIRECTION HYDRAULIC CONDUCTIVITY ... (PROP(1,2)) = 0.3500E+03
XY-DIRECTION HYDRAULIC CONDUCTIVITY .. (PROP(1,3)) = 0.0000E+00
SPECIFIC STORAGE ..... (PROP(1,4)) = 0.0000E+00
SATURATED WATER CONTENT..... (PROP(1,5)) = 0.4100E+00
AIR-ENTRY PRESSURE HEAD VALUE ..... (PROP(1,6)) = 0.0000E+00

```

```

MATERIAL NUMBER:    2  (1)

```

```

X-DIRECTION HYDRAULIC CONDUCTIVITY ... (PROP(1,1)) = 0.2500E+02

```

Y-DIRECTION HYDRAULIC CONDUCTIVITY ... (PROP(I,2)) = 0.2500E+02
 XY-DIRECTION HYDRAULIC CONDUCTIVITY .. (PROP(I,3)) = 0.0000E+00
 SPECIFIC STORAGE (PROP(I,4)) = 0.0000E+00
 SATURATED WATER CONTENT..... (PROP(I,5)) = 0.4300E+00
 AIR-ENTRY PRESSURE HEAD VALUE (PROP(I,6)) = 0.0000E+00

MATERIAL NUMBER: 3 (1)

X-DIRECTION HYDRAULIC CONDUCTIVITY ... (PROP(I,1)) = 0.1080E+02
 Y-DIRECTION HYDRAULIC CONDUCTIVITY ... (PROP(I,2)) = 0.1080E+02
 XY-DIRECTION HYDRAULIC CONDUCTIVITY .. (PROP(I,3)) = 0.0000E+00
 SPECIFIC STORAGE (PROP(I,4)) = 0.0000E+00
 SATURATED WATER CONTENT..... (PROP(I,5)) = 0.4500E+00
 AIR-ENTRY PRESSURE HEAD VALUE (PROP(I,6)) = 0.0000E+00

MATERIAL NUMBER: 1 (1)

RESIDUAL WATER SATURATION (PROP(I,7)) = 0.5740E-01
 POWER INDEX (N) OF K(REL) VS SAT..... (PROP(I,8)) = 0.1000E+01
 (SET N=-1 IF VAN GENUCHTEN REL. REQUIRED)
 COEFF (ALPHA) OF SAT. VS CAPIL. HEAD.. (PROP(I,9)) = 0.1240E+00
 POWER INDEX (BETA) (PROP(I,10))= 0.2280E+01
 POWER INDEX (GAMMA) (PROP(I,11))= 0.5614E+00

MATERIAL NUMBER: 2 (1)

RESIDUAL WATER SATURATION (PROP(I,7)) = 0.7740E-01
 POWER INDEX (N) OF K(REL) VS SAT..... (PROP(I,8)) = 0.1000E+01
 (SET N=-1 IF VAN GENUCHTEN REL. REQUIRED)
 COEFF (ALPHA) OF SAT. VS CAPIL. HEAD.. (PROP(I,9)) = 0.3600E-01
 POWER INDEX (BETA) (PROP(I,10))= 0.1560E+01
 POWER INDEX (GAMMA) (PROP(I,11))= 0.3590E+00

MATERIAL NUMBER: 3 (1)

RESIDUAL WATER SATURATION (PROP(I,7)) = 0.6750E-01
 POWER INDEX (N) OF K(REL) VS SAT..... (PROP(I,8)) = 0.1000E+01
 (SET N=-1 IF VAN GENUCHTEN REL. REQUIRED)
 COEFF (ALPHA) OF SAT. VS CAPIL. HEAD.. (PROP(I,9)) = 0.2000E-01
 POWER INDEX (BETA) (PROP(I,10))= 0.1410E+01
 POWER INDEX (GAMMA) (PROP(I,11))= 0.2908E+00

TRANSPORT PROPERTIES OF POROUS MEDIA

MATERIAL NUMBER: 1 (1)

LONGITUDINAL DISPERSIVITY ALPHA-L(PROPJ(I,1)) = 0.2000E+01
 TRANSVERSE DISPERSIVITY ALPHA-T(PROPJ(I,2)) = 0.2000E+01
 MOLECULAR DIFFUSION COMPONENT D-XX....(PROPJ(I,3)) = 0.0000E+00
 MOLECULAR DIFFUSION COMPONENT D-YY....(PROPJ(I,4)) = 0.0000E+00
 EFFECTIVE POROSITY(0 FOR STEADY STATE)(PROPJ(I,5)) = 0.4100E+00
 BULK DENSITY (g/cm**2)(PROPJ(I,6)) = 0.1650E+01

MATERIAL NUMBER: 2 (1)

LONGITUDINAL DISPERSIVITY ALPHA-L(PROPJ(I,1)) = 0.2000E+01
 TRANSVERSE DISPERSIVITY ALPHA-T(PROPJ(I,2)) = 0.2000E+01
 MOLECULAR DIFFUSION COMPONENT D-XX....(PROPJ(I,3)) = 0.0000E+00
 MOLECULAR DIFFUSION COMPONENT D-YY....(PROPJ(I,4)) = 0.0000E+00
 EFFECTIVE POROSITY(0 FOR STEADY STATE)(PROPJ(I,5)) = 0.4300E+00
 BULK DENSITY (g/cm**2)(PROPJ(I,6)) = 0.1550E+01

MATERIAL NUMBER: 3 (1)

LONGITUDINAL DISPERSIVITY ALPHA-L(PROPJ(I,1)) = 0.2000E+01
 TRANSVERSE DISPERSIVITY ALPHA-T(PROPJ(I,2)) = 0.2000E+01
 MOLECULAR DIFFUSION COMPONENT D-XX....(PROPJ(I,3)) = 0.0000E+00
 MOLECULAR DIFFUSION COMPONENT D-YY....(PROPJ(I,4)) = 0.0000E+00
 EFFECTIVE POROSITY(0 FOR STEADY STATE)(PROPJ(I,5)) = 0.4500E+00
 BULK DENSITY (g/cm**2)(PROPJ(I,6)) = 0.1500E+01

SOLUTE PROPERTIES

MATERIAL NUMBER: 1 (I)

DECAY COEFFICIENT (RPROP(I,1)) = 0.0000E+00

DISTRIBUTION COEFFICIENT (cm**3/g)... (RPROP(I,2)) = 0.0000E+00

MATERIAL NUMBER: 2 (I)

DECAY COEFFICIENT (RPROP(I,1)) = 0.0000E+00

DISTRIBUTION COEFFICIENT (cm**3/g)... (RPROP(I,2)) = 0.0000E+00

MATERIAL NUMBER: 3 (I)

DECAY COEFFICIENT (RPROP(I,1)) = 0.0000E+00

DISTRIBUTION COEFFICIENT (cm**3/g)... (RPROP(I,2)) = 0.0000E+00

X-COORDINATES OF GRID LINES

0.00	2.50	5.00	7.50	10.00	12.50	15.00	17.50
20.00	22.50	25.00	30.00	35.00	40.00	45.00	50.00

Y-COORDINATES OF GRID LINES

0.00	10.00	20.00	30.00	40.00	50.00	55.00	60.00
65.00	70.00	75.00	80.00	85.00	90.00	95.00	100.00

BOUNDARY CONDITION DATA

NUMBER OF STEADY DIRICHLET NODES (NBTO) = 32

NUMBER OF STEADY FLUX NODES (NDFLUX) = 0

NUMBER OF TRANSIENT DIRICHLET NODES (NBHVAR) = 0

NUMBER OF TRANSIENT FLUX NODES (NBFVAR) = 16

DIRICHLET BOUNDARY CONDITION DATA

INDEX	NODE NUMBER	DEP. VAR. #	PRESCRIBED VALUE
-------	-------------	-------------	------------------

1	1	1	-100.0
2	17	1	-100.0
3	33	1	-100.0
4	49	1	-100.0
5	65	1	-100.0
6	81	1	-100.0
7	97	1	-100.0
8	113	1	-100.0
9	129	1	-100.0
10	145	1	-100.0
11	161	1	-100.0
12	177	1	-100.0
13	193	1	-100.0
14	209	1	-100.0
15	225	1	-100.0
16	241	1	-100.0
17	16	2	1.000
18	32	2	1.000
19	48	2	1.000
20	64	2	1.000
21	80	2	1.000
22	96	2	1.000
23	112	2	1.000
24	128	2	1.000

25	144	2	1.000
26	160	2	1.000
27	176	2	1.000
28	192	2	1.000
29	208	2	1.000
30	224	2	1.000
31	240	2	1.000
32	256	2	1.000

TIME DEPENDENT FLUX B. C. FOR
 NODE # 16 DEPENDENT VARIABLE # 1

NUMBER OF CONTROL POINTS IN THE TIME GRAPH = 6
 TEMPORAL VARIATION (0=CONTINUOUS, 1=STEP) = 0

TIME VERSUS PRESCRIBED WATER FLUXES

0.0000E+00	0.0000E+00	1.000	12.50	2.000	10.00
3.000	0.0000E+00	4.000	0.0000E+00	50.00	0.0000E+00

TIME DEPENDENT FLUX B. C. FOR
 NODE # 32 DEPENDENT VARIABLE # 1

NUMBER OF CONTROL POINTS IN THE TIME GRAPH = 6
 TEMPORAL VARIATION (0=CONTINUOUS, 1=STEP) = 0

TIME VERSUS PRESCRIBED WATER FLUXES

0.0000E+00	0.0000E+00	1.000	25.00	2.000	20.00
3.000	0.0000E+00	4.000	0.0000E+00	50.00	0.0000E+00

TIME DEPENDENT FLUX B. C. FOR
 NODE # 48 DEPENDENT VARIABLE # 1

NUMBER OF CONTROL POINTS IN THE TIME GRAPH = 6
 TEMPORAL VARIATION (0=CONTINUOUS, 1=STEP) = 0

TIME VERSUS PRESCRIBED WATER FLUXES

0.0000E+00	0.0000E+00	1.000	25.00	2.000	20.00
3.000	0.0000E+00	4.000	0.0000E+00	50.00	0.0000E+00

TIME DEPENDENT FLUX B. C. FOR
 NODE # 64 DEPENDENT VARIABLE # 1

NUMBER OF CONTROL POINTS IN THE TIME GRAPH = 6
 TEMPORAL VARIATION (0=CONTINUOUS, 1=STEP) = 0

TIME VERSUS PRESCRIBED WATER FLUXES

0.0000E+00	0.0000E+00	1.000	25.00	2.000	20.00
3.000	0.0000E+00	4.000	0.0000E+00	50.00	0.0000E+00

TIME DEPENDENT FLUX B. C. FOR
 NODE # 80 DEPENDENT VARIABLE # 1

NUMBER OF CONTROL POINTS IN THE TIME GRAPH = 6
 TEMPORAL VARIATION (0=CONTINUOUS, 1=STEP) = 0

TIME VERSUS PRESCRIBED WATER FLUXES

0.0000E+00	0.0000E+00	1.000	25.00	2.000	20.00
3.000	0.0000E+00	4.000	0.0000E+00	50.00	0.0000E+00

TIME DEPENDENT FLUX B. C. FOR
 NODE # 96 DEPENDENT VARIABLE # 1

NUMBER OF CONTROL POINTS IN THE TIME GRAPH = 6
 TEMPORAL VARIATION (0=CONTINUOUS, 1=STEP) = 0

TIME VERSUS PRESCRIBED WATER FLUXES

0.0000E+00	0.0000E+00	1.000	25.00	2.000	20.00
3.000	0.0000E+00	4.000	0.0000E+00	50.00	0.0000E+00

TIME DEPENDENT FLUX B. C. FOR
 NODE # 112 DEPENDENT VARIABLE # 1

NUMBER OF CONTROL POINTS IN THE TIME GRAPH = 6
 TEMPORAL VARIATION (0=CONTINUOUS, 1=STEP) = 0

TIME VERSUS PRESCRIBED WATER FLUXES

0.0000E+00	0.0000E+00	1.000	25.00	2.000	20.00
3.000	0.0000E+00	4.000	0.0000E+00	50.00	0.0000E+00

TIME DEPENDENT FLUX B. C. FOR
 NODE # 128 DEPENDENT VARIABLE # 1

NUMBER OF CONTROL POINTS IN THE TIME GRAPH = 6
 TEMPORAL VARIATION (0=CONTINUOUS, 1=STEP) = 0

TIME VERSUS PRESCRIBED WATER FLUXES

0.0000E+00	0.0000E+00	1.000	25.00	2.000	20.00
3.000	0.0000E+00	4.000	0.0000E+00	50.00	0.0000E+00

TIME DEPENDENT FLUX B. C. FOR
 NODE # 144 DEPENDENT VARIABLE # 1

NUMBER OF CONTROL POINTS IN THE TIME GRAPH = 6
 TEMPORAL VARIATION (0=CONTINUOUS, 1=STEP) = 0

TIME VERSUS PRESCRIBED WATER FLUXES

0.0000E+00	0.0000E+00	1.000	25.00	2.000	20.00
3.000	0.0000E+00	4.000	0.0000E+00	50.00	0.0000E+00

TIME DEPENDENT FLUX B. C. FOR
 NODE # 160 DEPENDENT VARIABLE # 1

NUMBER OF CONTROL POINTS IN THE TIME GRAPH = 6
 TEMPORAL VARIATION (0=CONTINUOUS, 1=STEP) = 0

TIME VERSUS PRESCRIBED WATER FLUXES

0.0000E+00	0.0000E+00	1.000	25.00	2.000	20.00
3.000	0.0000E+00	4.000	0.0000E+00	50.00	0.0000E+00

TIME DEPENDENT FLUX B. C. FOR
 NODE # 176 DEPENDENT VARIABLE # 1

NUMBER OF CONTROL POINTS IN THE TIME GRAPH = 6
 TEMPORAL VARIATION (0=CONTINUOUS, 1=STEP) = 0

TIME VERSUS PRESCRIBED WATER FLUXES

0.0000E+00	0.0000E+00	1.000	37.50	2.000	30.00
3.000	0.0000E+00	4.000	0.0000E+00	50.00	0.0000E+00

TIME DEPENDENT FLUX B. C. FOR
 NODE # 192 DEPENDENT VARIABLE # 1

NUMBER OF CONTROL POINTS IN THE TIME GRAPH = 6
 TEMPORAL VARIATION (0=CONTINUOUS, 1=STEP) = 0

TIME VERSUS PRESCRIBED WATER FLUXES

0.0000E+00	0.0000E+00	1.000	50.00	2.000	40.00
3.000	0.0000E+00	4.000	0.0000E+00	50.00	0.0000E+00

TIME DEPENDENT FLUX B. C. FOR
 NODE # 208 DEPENDENT VARIABLE # 1

NUMBER OF CONTROL POINTS IN THE TIME GRAPH = 6
 TEMPORAL VARIATION (0=CONTINUOUS, 1=STEP) = 0

TIME VERSUS PRESCRIBED WATER FLUXES

0.0000E+00	0.0000E+00	1.000	50.00	2.000	40.00
3.000	0.0000E+00	4.000	0.0000E+00	50.00	0.0000E+00

TIME DEPENDENT FLUX B. C. FOR
 NODE # 224 DEPENDENT VARIABLE # 1

NUMBER OF CONTROL POINTS IN THE TIME GRAPH = 6
 TEMPORAL VARIATION (0=CONTINUOUS, 1=STEP) = 0

TIME VERSUS PRESCRIBED WATER FLUXES

0.0000E+00	0.0000E+00	1.000	50.00	2.000	40.00
3.000	0.0000E+00	4.000	0.0000E+00	50.00	0.0000E+00

TIME DEPENDENT FLUX B. C. FOR
NODE # 240 DEPENDENT VARIABLE # 1

NUMBER OF CONTROL POINTS IN THE TIME GRAPH = 6
TEMPORAL VARIATION (0=CONTINUOUS, 1=STEP) = 0

TIME VERSUS PRESCRIBED WATER FLUXES

0.0000E+00	0.0000E+00	1.000	50.00	2.000	40.00
3.000	0.0000E+00	4.000	0.0000E+00	50.00	0.0000E+00

TIME DEPENDENT FLUX B. C. FOR
NODE # 256 DEPENDENT VARIABLE # 1

NUMBER OF CONTROL POINTS IN THE TIME GRAPH = 6
TEMPORAL VARIATION (0=CONTINUOUS, 1=STEP) = 0

TIME VERSUS PRESCRIBED WATER FLUXES

0.0000E+00	0.0000E+00	1.000	25.00	2.000	20.00
3.000	0.0000E+00	4.000	0.0000E+00	50.00	0.0000E+00

DEFAULT VALUES AND WEIGHTING FACTORS

DEFAULT VALUE OF X-VELOCITY(VCX) = 0.0000E+00
DEFAULT VALUE OF Y-VELOCITY(VCY) = 0.0000E+00
X-DIRECTION UPSTREAM WEIGHTING FACTOR(WFAC) = 0.0000E+00
Y-DIRECTION UPSTREAM WEIGHTING FACTOR(YFAC) = 0.0000E+00
DEFAULT WATER SATURATION(SWD) = 0.0000E+00
STEADY-STATE VELOCITY FIELD (0=NO, 1=YES).(IVSTED) = 0

LIST OF BOUNDARY NODE NUMBERS:

1	16	17	32	33	48	49	64	65	80	81	96	97	112	113	128
129	144	145	160	161	176	177	192	193	208	209	224	225	240	241	256

----- ACTUAL HALF BAND WIDTH = 17 FULL BANDWIDTH = 35 -----

LIST OF OBSERVATION NODES

62 126 150 174 222

+++++ BEGIN TRANSIENT CALCULATIONS +++++

**** ELAPSED SIMULATION TIME : 0.5000 TIME STEP NUMBER : 1 TIME STEP SIZE: 0.500E+00 ****

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM ERROR	NODE NUMBER	RELAXATION FACTOR
1	240	-42.40	256	1.00
2	240	4.440	224	0.933
3	208	0.2076	23	1.00
4	0	-3.3737E-02	48	0.897

FLOW ANALYSIS IS COMPLETED FOR TARGET TIME STEP NO. 1 NUMBER OF COMPUTATIONAL TIME STEPS PERFORMED = 0

**** ELAPSED SIMULATION TIME : 1.000 TIME STEP NUMBER : 2 TIME STEP SIZE: 0.500E+00 ****

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM ERROR	NODE NUMBER	RELAXATION FACTOR
1	240	50.15	240	1.00
2	224	-9.925	192	0.876
3	112	0.2300	192	0.983
4	0	3.7496E-02	218	1.00

FLOW ANALYSIS IS COMPLETED FOR TARGET TIME STEP NO. 2 NUMBER OF COMPUTATIONAL TIME STEPS PERFORMED = 0

**** ELAPSED SIMULATION TIME : 1.500 TIME STEP NUMBER : 3 TIME STEP SIZE: 0.500E+00 ****

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM ERROR	NODE NUMBER	RELAXATION FACTOR
1	240	-17.98	240	1.00
2	208	2.344	240	0.917
3	0	-5.5409E-02	16	0.983

FLOW ANALYSIS IS COMPLETED FOR TARGET TIME STEP NO. 3 NUMBER OF COMPUTATIONAL TIME STEPS PERFORMED = 0

**** ELAPSED SIMULATION TIME : 2.000 TIME STEP NUMBER : 4 TIME STEP SIZE: 0.500E+00 ****

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM ERROR	NODE NUMBER	RELAXATION FACTOR
1	240	-5.342	208	1.00
2	192	0.9519	192	0.888
3	0	2.7004E-02	198	1.00

FLOW ANALYSIS IS COMPLETED FOR TARGET TIME STEP NO. 4 NUMBER OF COMPUTATIONAL TIME STEPS PERFORMED = 0

**** ELAPSED SIMULATION TIME : 2.500 TIME STEP NUMBER : 5 TIME STEP SIZE: 0.500E+00 ****

ITERATION	NUMBER OF NON-CONVERGENT NODES	MAXIMUM ERROR	NODE NUMBER	RELAXATION FACTOR
1	240	-24.66	64	1.00
2	192	1.710	64	0.955
3	0	3.9083E-02	22	1.00

*** NODAL FLUID FLUX VALUES ***

NODE	FLUID FLUX	NODE	FLUID FLUX	NODE	FLUID FLUX	NODE	FLUID FLUX	NODE	FLUID FLUX
1	-6.385	16	5.000	17	-12.77	32	10.00	33	-12.77
48	10.00	49	-12.77	64	10.00	65	-12.77	80	10.00
81	-12.77	96	10.00	97	-12.77	112	10.00	113	-12.77
128	10.00	129	-12.77	144	10.00	145	-12.77	160	10.00
161	-19.16	176	15.00	177	-25.54	192	20.00	193	-25.54
208	20.00	209	-25.54	224	20.00	225	-25.54	240	20.00
241	-12.77	256	10.00						

SUM OF ABOVE FLUX VALUES = -55.408

*** NODAL HEAD VALUES ***

NODE	HEAD VALUE	NODE	HEAD VALUE	NODE	HEAD VALUE	NODE	HEAD VALUE	NODE	HEAD VALUE
1	-100.0	2	-106.2	3	-112.1	4	-117.7	5	-123.1
6	-128.3	7	-130.8	8	-133.2	9	-135.7	10	-138.3
11	-140.9	12	-143.5	13	-146.2	14	-148.9	15	-150.6
16	-152.5	17	-100.0	18	-106.2	19	-112.1	20	-117.7
21	-123.1	22	-128.3	23	-130.8	24	-133.2	25	-135.7
26	-138.3	27	-140.9	28	-143.5	29	-146.2	30	-148.9
31	-150.6	32	-152.5	33	-100.0	34	-106.2	35	-112.1
36	-117.7	37	-123.1	38	-128.3	39	-130.8	40	-133.2
41	-135.7	42	-138.3	43	-140.9	44	-143.5	45	-146.2
46	-148.9	47	-150.6	48	-152.5	49	-100.0	50	-106.2
51	-112.1	52	-117.7	53	-123.1	54	-128.3	55	-130.8

56	-133.2	57	-135.7	58	-138.3	59	-140.9	60	-143.5
61	-146.2	62	-148.9	63	-150.6	64	-152.5	65	-100.0
66	-106.2	67	-112.1	68	-117.7	69	-123.1	70	-128.3
71	-130.8	72	-133.2	73	-135.7	74	-138.3	75	-140.9
76	-143.5	77	-146.2	78	-148.9	79	-150.6	80	-152.5
81	-100.0	82	-106.2	83	-112.1	84	-117.7	85	-123.1
86	-128.3	87	-130.8	88	-133.2	89	-135.7	90	-138.3
91	-140.9	92	-143.5	93	-146.2	94	-148.9	95	-150.6
96	-152.5	97	-100.0	98	-106.2	99	-112.1	100	-117.7
101	-123.1	102	-128.3	103	-130.8	104	-133.2	105	-135.7
106	-138.3	107	-140.9	108	-143.5	109	-146.2	110	-148.9
111	-150.6	112	-152.5	113	-100.0	114	-106.2	115	-112.1
116	-117.7	117	-123.1	118	-128.3	119	-130.8	120	-133.2
121	-135.7	122	-138.3	123	-140.9	124	-143.5	125	-146.2
126	-148.9	127	-150.6	128	-152.5	129	-100.0	130	-106.2
131	-112.1	132	-117.7	133	-123.1	134	-128.3	135	-130.8
136	-133.2	137	-135.7	138	-138.3	139	-140.9	140	-143.5
141	-146.2	142	-148.9	143	-150.6	144	-152.5	145	-100.0
146	-106.2	147	-112.1	148	-117.7	149	-123.1	150	-128.3
151	-130.8	152	-133.2	153	-135.7	154	-138.3	155	-140.9
156	-143.5	157	-146.2	158	-148.9	159	-150.6	160	-152.5
161	-100.0	162	-106.2	163	-112.1	164	-117.7	165	-123.1
166	-128.3	167	-130.8	168	-133.2	169	-135.7	170	-138.3
171	-140.9	172	-143.5	173	-146.2	174	-148.9	175	-150.6
176	-152.5	177	-100.0	178	-106.2	179	-112.1	180	-117.7
181	-123.1	182	-128.3	183	-130.8	184	-133.2	185	-135.7
186	-138.3	187	-140.9	188	-143.5	189	-146.2	190	-148.9
191	-150.6	192	-152.5	193	-100.0	194	-106.2	195	-112.1
196	-117.7	197	-123.1	198	-128.3	199	-130.8	200	-133.2
201	-135.7	202	-138.3	203	-140.9	204	-143.5	205	-146.2
206	-148.9	207	-150.6	208	-152.5	209	-100.0	210	-106.2
211	-112.1	212	-117.7	213	-123.1	214	-128.3	215	-130.8
216	-133.2	217	-135.7	218	-138.3	219	-140.9	220	-143.5
221	-146.2	222	-148.9	223	-150.6	224	-152.5	225	-100.0
226	-106.2	227	-112.1	228	-117.7	229	-123.1	230	-128.3
231	-130.8	232	-133.2	233	-135.7	234	-138.3	235	-140.9
236	-143.5	237	-146.2	238	-148.9	239	-150.6	240	-152.5
241	-100.0	242	-106.2	243	-112.1	244	-117.7	245	-123.1
246	-128.3	247	-130.8	248	-133.2	249	-135.7	250	-138.3
251	-140.9	252	-143.5	253	-146.2	254	-148.9	255	-150.6
256	-152.5								

*** LIST OF PARTIALLY SATURATED ELEMENTS ***

ELEM.	SAT. VALUE	ELEM.	SAT. VALUE	ELEM.	SAT. VALUE	ELEM.	SAT. VALUE	ELEM.	SAT. VALUE
1	0.0935	2	0.0910	3	0.0888	4	0.0870	5	0.0854
6	0.0844	7	0.0837	8	0.4478	9	0.4442	10	0.4407
11	0.4373	12	0.4338	13	0.4304	14	0.6298	15	0.6275
16	0.0935	17	0.0910	18	0.0888	19	0.0870	20	0.0854
21	0.0844	22	0.0837	23	0.4478	24	0.4442	25	0.4407
26	0.4373	27	0.4338	28	0.4304	29	0.6298	30	0.6275
31	0.0935	32	0.0910	33	0.0888	34	0.0870	35	0.0854
36	0.0844	37	0.0837	38	0.4478	39	0.4442	40	0.4407
41	0.4373	42	0.4338	43	0.4304	44	0.6298	45	0.6275
46	0.0935	47	0.0910	48	0.0888	49	0.0870	50	0.0854
51	0.0844	52	0.0837	53	0.4478	54	0.4442	55	0.4407
56	0.4373	57	0.4338	58	0.4304	59	0.6298	60	0.6275
61	0.0935	62	0.0910	63	0.0888	64	0.0870	65	0.0854
66	0.0844	67	0.0837	68	0.4478	69	0.4442	70	0.4407
71	0.4373	72	0.4338	73	0.4304	74	0.6298	75	0.6275
76	0.0935	77	0.0910	78	0.0888	79	0.0870	80	0.0854
81	0.0844	82	0.0837	83	0.4478	84	0.4442	85	0.4407
86	0.4373	87	0.4338	88	0.4304	89	0.6298	90	0.6275
91	0.0935	92	0.0910	93	0.0888	94	0.0870	95	0.0854
96	0.0844	97	0.0837	98	0.4478	99	0.4442	100	0.4407
101	0.4373	102	0.4338	103	0.4304	104	0.6298	105	0.6275
106	0.0935	107	0.0910	108	0.0888	109	0.0870	110	0.0854
111	0.0844	112	0.0837	113	0.4478	114	0.4442	115	0.4407

116	0.4373	117	0.4338	118	0.4304	119	0.6298	120	0.6275
121	0.0935	122	0.0910	123	0.0888	124	0.0870	125	0.0854
126	0.0844	127	0.0837	128	0.4478	129	0.4442	130	0.4407
131	0.4373	132	0.4338	133	0.4304	134	0.6298	135	0.6275
136	0.0935	137	0.0910	138	0.0888	139	0.0870	140	0.0854
141	0.0844	142	0.0837	143	0.4478	144	0.4442	145	0.4407
146	0.4373	147	0.4338	148	0.4304	149	0.6298	150	0.6275
151	0.0935	152	0.0910	153	0.0888	154	0.0870	155	0.0854
156	0.0844	157	0.0837	158	0.4478	159	0.4442	160	0.4407
161	0.4373	162	0.4338	163	0.4304	164	0.6298	165	0.6275
166	0.0935	167	0.0910	168	0.0888	169	0.0870	170	0.0854
171	0.0844	172	0.0837	173	0.4478	174	0.4442	175	0.4407
176	0.4373	177	0.4338	178	0.4304	179	0.6298	180	0.6275
181	0.0935	182	0.0910	183	0.0888	184	0.0870	185	0.0854
186	0.0844	187	0.0837	188	0.4478	189	0.4442	190	0.4407
191	0.4373	192	0.4338	193	0.4304	194	0.6298	195	0.6275
196	0.0935	197	0.0910	198	0.0888	199	0.0870	200	0.0854
201	0.0844	202	0.0837	203	0.4478	204	0.4442	205	0.4407
206	0.4373	207	0.4338	208	0.4304	209	0.6298	210	0.6275
211	0.0935	212	0.0910	213	0.0888	214	0.0870	215	0.0854
216	0.0844	217	0.0837	218	0.4478	219	0.4442	220	0.4407
221	0.4373	222	0.4338	223	0.4304	224	0.6298	225	0.6275

*** ELEMENTAL FLUID VELOCITY ***

ELEMENT	X-VELOCITY	Y-VELOCITY	ELEMENT	X-VELOCITY	Y-VELOCITY	ELEMENT	X-VELOCITY	Y-VELOCITY
1	0.000E+00	-5.11	2	0.000E+00	-5.10	3	6.633E-14	-5.09
4	6.246E-14	-5.07	5	0.000E+00	-5.04	6	0.000E+00	-5.02
7	0.000E+00	-5.01	8	5.705E-14	-4.95	9	1.130E-13	-4.85
10	5.596E-14	-4.75	11	0.000E+00	-4.63	12	0.000E+00	-4.51
13	0.000E+00	-4.38	14	3.702E-14	-4.25	15	3.687E-14	-4.09
16	-7.622E-14	-5.11	17	-7.085E-14	-5.10	18	1.327E-13	-5.09
19	1.249E-13	-5.07	20	-5.913E-14	-5.04	21	-1.138E-13	-5.02
22	-1.111E-13	-5.01	23	-5.705E-14	-4.95	24	0.000E+00	-4.85
25	5.596E-14	-4.75	26	5.543E-14	-4.63	27	-5.490E-14	-4.51
28	5.438E-14	-4.38	29	1.111E-13	-4.25	30	1.106E-13	-4.09
31	0.000E+00	-5.11	32	2.126E-13	-5.10	33	2.653E-13	-5.09
34	1.249E-13	-5.07	35	5.913E-14	-5.04	36	0.000E+00	-5.02
37	0.000E+00	-5.01	38	-1.141E-13	-4.95	39	-1.130E-13	-4.85
40	5.596E-14	-4.75	41	0.000E+00	-4.63	42	0.000E+00	-4.51
43	5.438E-14	-4.38	44	3.702E-14	-4.25	45	0.000E+00	-4.09
46	7.622E-14	-5.11	47	1.417E-13	-5.10	48	1.327E-13	-5.09
49	2.498E-13	-5.07	50	5.913E-14	-5.04	51	-1.138E-13	-5.02
52	-1.666E-13	-5.01	53	-1.712E-13	-4.95	54	-5.650E-14	-4.85
55	-1.119E-13	-4.75	56	-5.543E-14	-4.63	57	5.490E-14	-4.51
58	1.631E-13	-4.38	59	1.851E-13	-4.25	60	1.475E-13	-4.09
61	1.524E-13	-5.11	62	2.126E-13	-5.10	63	1.327E-13	-5.09
64	1.249E-13	-5.07	65	5.913E-14	-5.04	66	-5.688E-14	-5.02
67	-2.221E-13	-5.01	68	-1.712E-13	-4.95	69	-2.260E-13	-4.85
70	-1.119E-13	-4.75	71	1.109E-13	-4.63	72	1.098E-13	-4.51
73	1.631E-13	-4.38	74	1.111E-13	-4.25	75	1.475E-13	-4.09
76	2.287E-13	-5.11	77	3.543E-13	-5.10	78	2.653E-13	-5.09
79	1.249E-13	-5.07	80	1.183E-13	-5.04	81	0.000E+00	-5.02
82	-1.666E-13	-5.01	83	-1.712E-13	-4.95	84	-5.650E-14	-4.85
85	0.000E+00	-4.75	86	5.543E-14	-4.63	87	1.647E-13	-4.51
88	1.088E-13	-4.38	89	7.403E-14	-4.25	90	1.106E-13	-4.09
91	2.287E-13	-5.11	92	3.543E-13	-5.10	93	2.653E-13	-5.09
94	1.249E-13	-5.07	95	1.183E-13	-5.04	96	1.138E-13	-5.02
97	0.000E+00	-5.01	98	-2.282E-13	-4.95	99	-1.695E-13	-4.85
100	5.596E-14	-4.75	101	1.109E-13	-4.63	102	0.000E+00	-4.51
103	-1.088E-13	-4.38	104	1.111E-13	-4.25	105	2.212E-13	-4.09
106	1.524E-13	-5.11	107	2.834E-13	-5.10	108	1.327E-13	-5.09
109	0.000E+00	-5.07	110	1.183E-13	-5.04	111	2.275E-13	-5.02
112	5.553E-14	-5.01	113	-5.705E-14	-4.95	114	0.000E+00	-4.85
115	0.000E+00	-4.75	116	0.000E+00	-4.63	117	0.000E+00	-4.51
118	0.000E+00	-4.38	119	-3.702E-14	-4.25	120	3.687E-14	-4.09
121	0.000E+00	-5.11	122	2.126E-13	-5.10	123	2.653E-13	-5.09
124	1.249E-13	-5.07	125	1.183E-13	-5.04	126	1.706E-13	-5.02

127	5.553E-14	-5.01	128	-5.705E-14	-4.95	129	-1.130E-13	-4.85
130	-1.679E-13	-4.75	131	-1.663E-13	-4.63	132	-1.098E-13	-4.51
133	-5.438E-14	-4.38	134	7.403E-14	-4.25	135	7.374E-14	-4.09
136	0.000E+00	-5.11	137	1.417E-13	-5.10	138	2.653E-13	-5.09
139	1.249E-13	-5.07	140	0.000E+00	-5.04	141	5.688E-14	-5.02
142	1.111E-13	-5.01	143	1.141E-13	-4.95	144	-5.650E-14	-4.85
145	-1.679E-13	-4.75	146	-1.109E-13	-4.63	147	-5.490E-14	-4.51
148	0.000E+00	-4.38	149	-3.702E-14	-4.25	150	0.000E+00	-4.09
151	3.811E-14	-5.11	152	1.063E-13	-5.10	153	1.990E-13	-5.09
154	9.369E-14	-5.07	155	-5.913E-14	-5.04	156	-2.844E-14	-5.02
157	1.388E-13	-5.01	158	1.426E-13	-4.95	159	0.000E+00	-4.85
160	-1.679E-13	-4.75	161	-1.386E-13	-4.63	162	8.235E-14	-4.51
163	8.156E-14	-4.38	164	-1.851E-14	-4.25	165	-7.374E-14	-4.09
166	-3.811E-14	-5.11	167	3.543E-14	-5.10	168	6.633E-14	-5.09
169	3.123E-14	-5.07	170	2.956E-14	-5.04	171	0.000E+00	-5.02
172	-2.776E-14	-5.01	173	-5.705E-14	-4.95	174	-1.130E-13	-4.85
175	-2.798E-14	-4.75	176	0.000E+00	-4.63	177	-1.098E-13	-4.51
178	-1.359E-13	-4.38	179	-5.553E-14	-4.25	180	0.000E+00	-4.09
181	7.622E-14	-5.11	182	7.085E-14	-5.10	183	3.316E-14	-5.09
184	3.123E-14	-5.07	185	2.956E-14	-5.04	186	0.000E+00	-5.02
187	-5.553E-14	-5.01	188	-1.997E-13	-4.95	189	-2.260E-13	-4.85
190	-1.959E-13	-4.75	191	-1.386E-13	-4.63	192	-1.098E-13	-4.51
193	-5.438E-14	-4.38	194	0.000E+00	-4.25	195	0.000E+00	-4.09
196	0.000E+00	-5.11	197	0.000E+00	-5.10	198	3.316E-14	-5.09
199	3.123E-14	-5.07	200	-2.956E-14	-5.04	201	-5.688E-14	-5.02
202	-8.329E-14	-5.01	203	-5.705E-14	-4.95	204	-2.825E-14	-4.85
205	-5.596E-14	-4.75	206	-8.314E-14	-4.63	207	-2.745E-14	-4.51
208	-2.719E-14	-4.38	209	-1.851E-14	-4.25	210	0.000E+00	-4.09
211	0.000E+00	-5.11	212	0.000E+00	-5.10	213	0.000E+00	-5.09
214	3.123E-14	-5.07	215	-2.956E-14	-5.04	216	-8.532E-14	-5.02
217	-2.776E-14	-5.01	218	5.705E-14	-4.95	219	5.650E-14	-4.85
220	2.798E-14	-4.75	221	5.543E-14	-4.63	222	0.000E+00	-4.51
223	-8.156E-14	-4.38	224	-7.403E-14	-4.25	225	-3.687E-14	-4.09

FLOW ANALYSIS IS COMPLETED FOR TARGET TIME STEP NO. 5 NUMBER OF COMPUTATIONAL TIME STEPS PERFORMED = 0

*** VOLUMETRIC FLOW BALANCE INFORMATION AT TIME = 0.2500E+01***

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

NET FLOW RATE DUE TO BOUNDARY FLUX AND SINKS -55.408
 RATE OF FLUID ACCUMULATION -58.559
 MASS BALANCE ERROR 3.1501
 NORMALIZED MASS BALANCE ERROR 6.12901E-03
 CUMULATIVE FLUID STORAGE -73.844

*** NODAL DISPERSIVE FLUX VALUES ***

NODE	DISP. FLUX	NODE	DISP. FLUX	NODE	DISP. FLUX	NODE	DISP. FLUX	NODE	DISP. FLUX
1	-1.8319E-15	16	6.8543E-04	17	-4.7740E-15	32	1.3709E-03	33	-1.1102E-16
48	1.3709E-03	49	-3.4417E-15	64	1.3709E-03	65	2.2204E-16	80	1.3709E-03
81	5.5511E-15	96	1.3709E-03	97	-2.2204E-15	112	1.3709E-03	113	-1.7764E-15
128	1.3709E-03	129	3.1086E-15	144	1.3709E-03	145	-7.7716E-16	160	1.3709E-03
161	-5.9952E-15	176	2.0563E-03	177	1.9984E-15	192	2.7417E-03	193	1.0436E-14
208	2.7417E-03	209	-1.7764E-15	224	2.7417E-03	225	6.6613E-16	240	2.7417E-03
241	3.3307E-16	256	1.3709E-03						

SUM OF ABOVE FLUX VALUES = 2.74171E-02

*** INCREMENTAL MASS BALANCE RESULTS OVER A TIME STEP ***

TOTAL DISPERSIVE FLUX RATE	2.74171E-02
TOTAL ADVECTIVE FLUX RATE	-9.5146
TOTAL DISPERSIVE + ADVECTIVE FLUX RATE	-9.4872
RATE OF MASS DECAY AND TRANSFORMATION	0.00000E+00
NET RATE OF MATERIAL ACCUMULATION	-9.5508
MASS BALANCE ERROR	6.35852E-02
NORMALIZED MASS BALANCE ERROR	1.34620E-04
RATE OF MASS ACCUMULATION DUE TO PRESSURE HEAD CHANGE	-53.239

*** CUMULATIVE MASS BALANCE RESULTS ***

CUMULATIVE MATERIAL STORAGE	492.45
CUMULATIVE MASS DECAY AND TRANSFORMATION.....	0.00000E+00

*** NODAL CONCENTRATION VALUES ***

NODE	CONC. VALUE	NODE	CONC. VALUE	NODE	CONC. VALUE	NODE	CONC. VALUE	NODE	CONC. VALUE
1	0.8203	2	0.8311	3	0.8473	4	0.8598	5	0.8726
6	0.8841	7	0.8896	8	0.8950	9	0.9129	10	0.9397
11	0.9601	12	0.9755	13	0.9863	14	0.9931	15	0.9978
16	1.000	17	0.8203	18	0.8311	19	0.8473	20	0.8598
21	0.8726	22	0.8841	23	0.8896	24	0.8950	25	0.9129
26	0.9397	27	0.9601	28	0.9755	29	0.9863	30	0.9931
31	0.9978	32	1.000	33	0.8203	34	0.8311	35	0.8473
36	0.8598	37	0.8726	38	0.8841	39	0.8896	40	0.8950
41	0.9129	42	0.9397	43	0.9601	44	0.9755	45	0.9863
46	0.9931	47	0.9978	48	1.000	49	0.8203	50	0.8311
51	0.8473	52	0.8598	53	0.8726	54	0.8841	55	0.8896
56	0.8950	57	0.9129	58	0.9397	59	0.9601	60	0.9755
61	0.9863	62	0.9931	63	0.9978	64	1.000	65	0.8203
66	0.8311	67	0.8473	68	0.8598	69	0.8726	70	0.8841
71	0.8896	72	0.8950	73	0.9129	74	0.9397	75	0.9601
76	0.9755	77	0.9863	78	0.9931	79	0.9978	80	1.000
81	0.8203	82	0.8311	83	0.8473	84	0.8598	85	0.8726
86	0.8841	87	0.8896	88	0.8950	89	0.9129	90	0.9397
91	0.9601	92	0.9755	93	0.9863	94	0.9931	95	0.9978
96	1.000	97	0.8203	98	0.8311	99	0.8473	100	0.8598
101	0.8726	102	0.8841	103	0.8896	104	0.8950	105	0.9129
106	0.9397	107	0.9601	108	0.9755	109	0.9863	110	0.9931
111	0.9978	112	1.000	113	0.8203	114	0.8311	115	0.8473
116	0.8598	117	0.8726	118	0.8841	119	0.8896	120	0.8950
121	0.9129	122	0.9397	123	0.9601	124	0.9755	125	0.9863
126	0.9931	127	0.9978	128	1.000	129	0.8203	130	0.8311
131	0.8473	132	0.8598	133	0.8726	134	0.8841	135	0.8896
136	0.8950	137	0.9129	138	0.9397	139	0.9601	140	0.9755
141	0.9863	142	0.9931	143	0.9978	144	1.000	145	0.8203
146	0.8311	147	0.8473	148	0.8598	149	0.8726	150	0.8841
151	0.8896	152	0.8950	153	0.9129	154	0.9397	155	0.9601
156	0.9755	157	0.9863	158	0.9931	159	0.9978	160	1.000
161	0.8203	162	0.8311	163	0.8473	164	0.8598	165	0.8726
166	0.8841	167	0.8896	168	0.8950	169	0.9129	170	0.9397
171	0.9601	172	0.9755	173	0.9863	174	0.9931	175	0.9978
176	1.000	177	0.8203	178	0.8311	179	0.8473	180	0.8598
181	0.8726	182	0.8841	183	0.8896	184	0.8950	185	0.9129
186	0.9397	187	0.9601	188	0.9755	189	0.9863	190	0.9931
191	0.9978	192	1.000	193	0.8203	194	0.8311	195	0.8473
196	0.8598	197	0.8726	198	0.8841	199	0.8896	200	0.8950
201	0.9129	202	0.9397	203	0.9601	204	0.9755	205	0.9863

206	0.9931	207	0.9978	208	1.000	209	0.8203	210	0.8311
211	0.8473	212	0.8598	213	0.8726	214	0.8841	215	0.8896
216	0.8950	217	0.9129	218	0.9397	219	0.9601	220	0.9755
221	0.9863	222	0.9931	223	0.9978	224	1.000	225	0.8203
226	0.8311	227	0.8473	228	0.8598	229	0.8726	230	0.8841
231	0.8896	232	0.8950	233	0.9129	234	0.9397	235	0.9601
236	0.9755	237	0.9863	238	0.9931	239	0.9978	240	1.000
241	0.8203	242	0.8311	243	0.8473	244	0.8598	245	0.8726
246	0.8841	247	0.8896	248	0.8950	249	0.9129	250	0.9397
251	0.9601	252	0.9755	253	0.9863	254	0.9931	255	0.9978
256	1.000								

*** OBSERVATION NODE INFORMATION ***

NODAL VALUES OF DEPENDENT VARIABLE OVER TIME

OBSERVED NODE NUMBER: 62

TIME	HEAD VALUE	TIME	HEAD VALUE	TIME	HEAD VALUE	TIME	HEAD VALUE
----	-----	----	-----	----	-----	----	-----
0.5000E+00	-0.1360E+03	0.1000E+01	-0.1195E+03	0.1500E+01	-0.1210E+03	0.2000E+01	-0.1262E+03
0.2500E+01	-0.1489E+03						

OBSERVED NODE NUMBER: 126

TIME	HEAD VALUE	TIME	HEAD VALUE	TIME	HEAD VALUE	TIME	HEAD VALUE
----	-----	----	-----	----	-----	----	-----
0.5000E+00	-0.1360E+03	0.1000E+01	-0.1195E+03	0.1500E+01	-0.1210E+03	0.2000E+01	-0.1262E+03
0.2500E+01	-0.1489E+03						

OBSERVED NODE NUMBER: 150

TIME	HEAD VALUE	TIME	HEAD VALUE	TIME	HEAD VALUE	TIME	HEAD VALUE
----	-----	----	-----	----	-----	----	-----
0.5000E+00	-0.1209E+03	0.1000E+01	-0.1139E+03	0.1500E+01	-0.1142E+03	0.2000E+01	-0.1168E+03
0.2500E+01	-0.1283E+03						

OBSERVED NODE NUMBER: 174

TIME	HEAD VALUE	TIME	HEAD VALUE	TIME	HEAD VALUE	TIME	HEAD VALUE
----	-----	----	-----	----	-----	----	-----
0.5000E+00	-0.1360E+03	0.1000E+01	-0.1195E+03	0.1500E+01	-0.1210E+03	0.2000E+01	-0.1262E+03
0.2500E+01	-0.1489E+03						

OBSERVED NODE NUMBER: 222

TIME	HEAD VALUE	TIME	HEAD VALUE	TIME	HEAD VALUE	TIME	HEAD VALUE
----	-----	----	-----	----	-----	----	-----
0.5000E+00	-0.1360E+03	0.1000E+01	-0.1195E+03	0.1500E+01	-0.1210E+03	0.2000E+01	-0.1262E+03
0.2500E+01	-0.1489E+03						

OBSERVED NODE NUMBER: 62

TIME	CONCENTRATION	TIME	CONCENTRATION	TIME	CONCENTRATION	TIME	CONCENTRATION
----	-----	----	-----	----	-----	----	-----
0.5000E+00	0.4118E+00	0.1000E+01	0.8178E+00	0.1500E+01	0.9469E+00	0.2000E+01	0.9841E+00
0.2500E+01	0.9931E+00						

OBSERVED NODE NUMBER: 126

TIME	CONCENTRATION	TIME	CONCENTRATION	TIME	CONCENTRATION	TIME	CONCENTRATION
----	-----	----	-----	----	-----	----	-----
0.5000E+00	0.4118E+00	0.1000E+01	0.8178E+00	0.1500E+01	0.9469E+00	0.2000E+01	0.9841E+00
0.2500E+01	0.9931E+00						

OBSERVED NODE NUMBER: 150

TIME	CONCENTRATION	TIME	CONCENTRATION	TIME	CONCENTRATION	TIME	CONCENTRATION
----	-----	----	-----	----	-----	----	-----
0.5000E+00	0.7407E-01	0.1000E+01	0.3464E+00	0.1500E+01	0.6216E+00	0.2000E+01	0.8038E+00
0.2500E+01	0.8841E+00						

OBSERVED NODE NUMBER: 174

TIME	CONCENTRATION	TIME	CONCENTRATION	TIME	CONCENTRATION	TIME	CONCENTRATION
----	-----	----	-----	----	-----	----	-----
0.5000E+00	0.4118E+00	0.1000E+01	0.8178E+00	0.1500E+01	0.9469E+00	0.2000E+01	0.9841E+00
0.2500E+01	0.9931E+00						

OBSERVED NODE NUMBER: 222

TIME	CONCENTRATION	TIME	CONCENTRATION	TIME	CONCENTRATION	TIME	CONCENTRATION
----	-----	----	-----	----	-----	----	-----
0.5000E+00	0.4118E+00	0.1000E+01	0.8178E+00	0.1500E+01	0.9469E+00	0.2000E+01	0.9841E+00
0.2500E+01	0.9931E+00						

***** VAM2D HAS FULLY EXECUTED *****

10.5 PROBLEM 4: CHAIN DECAY TRANSPORT SIMULATION

10.5.1 Input Data

The input data file for this sample multi-component transport problem is presented in Table 10.7. Note that the modeling option parameters IMODL and ICHAIN are set to 0 and 1, respectively. This indicates that chain decay transport simulation is required. Solute transport parameters for multi-species simulation are specified via record group 11c. The input data also includes the specification of two decaying source node boundary conditions and source characteristics via record groups 15 and 17. Output concentration values are to be written every third timestep (NSTEP=3).

10.5.2 Sample Output

Output of the transport calculation is displayed in Table 10.8. This output consists of the following categories of information:

1. Brief summary of control input parameters and material properties.
2. Mesh data.
3. Boundary condition data.
4. Decaying source data and related boundary conditions.
5. Element numbers and centroidal coordinates.
6. List of observation nodes and monitored specie component numbers.
7. Mass balance summary for each specie component.
8. Concentration values for each specie component.

Table 10.7. Input for the 1-D Chain Decay Transport Problems.

ONE DIMENSIONAL TRANSPORT OF A THREE-MEMBER STRAIGHT CHAIN														GROUP1
0	0	0	0	1	0	1	15	42	20	0	0	1	0	GROUP2
0	0	1	0	0	0	0.0	0.0	0.0	0	0	0			GROUP3
0	0	0	0	0	0	0	3	1	1	0	0			GROUP4
	0.0	18.2		1.0		18.2								GROUP5
	0.0	0.0												GROUP6A
	8.5	8.5		0.0		0.0		0.1		2.34				GROUP7
3	1													GROUP11A
1														GROUP11C
1	3	1	2	3										
1	0													
2	1													
1		1.0												
3	1													
2		1.0												
1	0													
0.16E-2		4.62E-2	1.06E-4											
4.00E2		4.00E2	4.00E2											
2	21	32.8	2.0	0										
	32.8	2.0	656.0			2.0		1.0		1.0		.0.0	0.0	GROUP12
0	0	0	0	2										GROUP14
1														GROUP15A
1	1.0E06													GROUP17A
0.16E-2		4.62E-2	1.06E-4											
1	1	2	239.4											GROUP17B
	239.4		0.0	0.0										
2	1	2	239.4											
	239.4		0.0	0.0										
	239.4		0.0	0.10		0.0		1.0	1					GROUP19
4														GROUP23A
1	2	41	42											GROUP23B
	239.4	239.4	-239.4	-239.4										GROUP23C
3														GROUP27
19	19	19												
1	2	3												

Table 10.8. Sample Output for the 1-D Chain Decay Transport Problem.

```

*****
                        THIS OUTPUT GENERATED BY VAM2D v. 5.2
                        INPUT FILE NAME = tbl10.7
*****

NUMBER OF PROBLEMS TO BE SOLVED = 1

PROBLEM NUMBER: 1

PROBLEM TITLE
-----
ONE DIMENSIONAL TRANSPORT OF A THREE-MEMBER STRAIGHT CHAIN
-----

PROBLEM SPECIFICATION PARAMETERS
-----
MODEL OPTION PARAMETER .....(IMODL) = 0
  NOTE: IMODL = 0 FOR SOLUTE TRANSPORT ONLY
           = 1 FOR WATER FLOW ONLY
           = 2 FOR COUPLED FLOW AND TRANSPORT
HYSTERETIC SOIL MOISTURE (1=YES, 0=NO)....(IHYST) = 0
ANISOTROPIC REL. COND.(1=YES, 0=NO).....(IANI) = 0
CONVERT INITIAL HEAD VALUES(1=YES, 0=NO).(INTSPC) = 0
CHAIN-DECAY REACTIONS(1=YES, 0=NO).....(ICHAIN) = 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) = 15
TOTAL NUMBER OF NODES .....(NP) = 42
TOTAL NUMBER OF ELEMENTS .....(NE) = 20
SEQUENTIAL NUMBERING INDEX (0=Y, 1=X-DIR) (ISWAP) = 0
AXISYMMETRIC SIMULATION(1=YES, 0=NO).....(IAXSYM) = 0
NUMBER OF POROUS MATRIX MATERIALS .....(NMAT) = 1
INITIAL CONDITION NON-UNIFORMITY INDEX.....(NONU) = 0
NUMBER OF INFIL./EVAP. ELEMENTS .....(NEIEVP) = 0
NUMBER PLANT SPECIES .....(NPLANT) = 0

TIME STEPPING AND ITERATION CONTROL PARAMETERS
-----
TIME STEPPING INDEX (0=CNTRL, 1=BCKWD) ...(IKALL) = 0
TYPE OF ITERATION SCHEME (1=NEWT,0=PICARD)(INEWT) = 0
MAXIMUM NON-LINEAR ITERATIONS .....(NITMAX) = 1
MAXIMUM NUMBER OF TIME STEP REFINEMENTS ..(IRESOL) = 0
LUMPING OF ELEMENT MATRIX (1=YES, 0=NO) ..(ILUMP) = 0

INPUT / OUTPUT CONTROL PARAMETERS
-----
VELOCITY/SATURATION INPUT.....(NVREAD) = 0
BOUNDARY NODE DATA READ (1=YES, 0=NO)....(IOUTLT) = 0
NUMBER OF NODES FOR WHICH I.C. ARE READ....(NPIN) = 0
OUTPUT REQUIREMENT INDICATOR:
  (0=ALL DATA, 1=NO ELEMENT DATA,
   2=NO DATA, 3=NO MESH AND I.C. DATA.....(IPRD) = 0
UNIT 9 OUTPUT OF VEL / SAT (1=YES, 0=NO).(NVWRIT) = 0
VELOCITY PRINTOUT CONTROL INDEX.....(NVPR) = 0

```

UNIT 10 OUTPUT HEAD/CONC. (0=NONE, N=NTH).(NPLOT) = 0
 NODAL VALUE PRINTOUT CONTROL INDEX.....(NSTEP) = 3
 OBSERVATION MODE INDEX.....(IOBSND) = 1
 MASS BALANCE TO BE PERFORMED (1=YES,0=NO).(IMBAL) = 1
 UNIT 8 OUTPUT OF HEAD/CONC (1=YES, 0=NO).(NOWRIT) = 0
 PRINT CHECK OPTION INDEX.....(IPRCHK) = 0

TEMPORAL DISCRETIZATION DATA

 INITIAL TIME VALUE (TIMA) = 0.0000E+00
 VALUE OF FIRST TIME STEP (TIN) = 0.1820E+02
 TIME STEP MULTIPLIER (TFAC) = 0.1000E+01
 MAXIMUM TIME STEP SIZE (TMAX) = 0.1820E+02

*** LIST OF GENERATED TIME VALUES ***

 0.182E+02 0.364E+02 0.546E+02 0.728E+02 0.910E+02 0.109E+03 0.127E+03 0.146E+03
 0.164E+03 0.182E+03 0.200E+03 0.218E+03 0.237E+03 0.255E+03 0.273E+03

DEFAULT INITIAL CONCENTRATION VALUE

 0.0000E+00

TRANSPORT PROPERTIES OF POROUS MEDIA

 MATERIAL NUMBER: 1 (I)

LONGITUDINAL DISPERSIVITY ALPHA-L(PROPJ(1,1)) = 0.8500E+01
 TRANSVERSE DISPERSIVITY ALPHA-T(PROPJ(1,2)) = 0.8500E+01
 MOLECULAR DIFFUSION COMPONENT D-XX....(PROPJ(1,3)) = 0.0000E+00
 MOLECULAR DIFFUSION COMPONENT D-YY....(PROPJ(1,4)) = 0.0000E+00
 EFFECTIVE POROSITY(0 FOR STEADY STATE)(PROPJ(1,5)) = 0.1000E+00
 BULK DENSITY (g/cm**2)(PROPJ(1,6)) = 0.2340E+01

SOLUTE DATA FOR DECAY CHAIN MODELING

 NUMBER OF SPECIE COMPONENTS = 3

DECAYING SOURCE BOUNDARY CONDITION INDEX = 1

REACTION PATH DATA

 NUMBER OF DECAY CHAINS OR REACTION PATHS = 1

REACTION PATH NUMBER = 1

NUMBER OF COMPONENTS IN THE PATH = 3

LIST OF COMPONENT NUMBERS

 1 2 3

SPECIES TRANSFORMATION DATA

 SPECIES COMPONENT NUMBER = 1

NUMBER OF IMMEDIATE PARENTS = 0

SPECIES TRANSFORMATION DATA

 SPECIES COMPONENT NUMBER = 2

NUMBER OF IMMEDIATE PARENTS = 1

LIST OF PARENT-SPECIES COMPONENT NUMBER AND TRANS. MASS FRACTION

1 0.100E+01

SPECIES TRANSFORMATION DATA

SPECIES COMPONENT NUMBER = 3
NUMBER OF IMMEDIATE PARENTS = 1

LIST OF PARENT-SPECIES COMPONENT NUMBER AND TRANS. MASS FRACTION

2 0.100E+01

DECAY AND DISTRIBUTION COEFF. DATA

SOIL MATERIAL NUMBER = 1

SOLUTE SPECIES COMPONENT NUMBER = 1
DECAY COEFFICIENT VALUE = 0.160E-02
DISTRIBUTION COEFFICIENT VALUE = 0.400E+03

SOLUTE SPECIES COMPONENT NUMBER = 2
DECAY COEFFICIENT VALUE = 0.462E-01
DISTRIBUTION COEFFICIENT VALUE = 0.400E+03

SOLUTE SPECIES COMPONENT NUMBER = 3
DECAY COEFFICIENT VALUE = 0.106E-03
DISTRIBUTION COEFFICIENT VALUE = 0.400E+03

*** FINITE-ELEMENT MESH CONNECTIONS ***

(NUMBERING IS COUNTER-CLOCKWISE)

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

*** NODAL COORDINATES ***

NODE	X-COOR.	Y-COOR.	NODE	X-COOR.	Y-COOR.	NODE	X-COOR.	Y-COOR.
----	-----	-----	----	-----	-----	----	-----	-----
1	0.00	0.00	2	0.00	2.00	3	32.80	0.00
4	32.80	2.00	5	65.60	0.00	6	65.60	2.00
7	98.40	0.00	8	98.40	2.00	9	131.20	0.00
10	131.20	2.00	11	164.00	0.00	12	164.00	2.00
13	196.80	0.00	14	196.80	2.00	15	229.60	0.00
16	229.60	2.00	17	262.40	0.00	18	262.40	2.00
19	295.20	0.00	20	295.20	2.00	21	328.00	0.00
22	328.00	2.00	23	360.80	0.00	24	360.80	2.00
25	393.60	0.00	26	393.60	2.00	27	426.40	0.00
28	426.40	2.00	29	459.20	0.00	30	459.20	2.00
31	492.00	0.00	32	492.00	2.00	33	524.80	0.00
34	524.80	2.00	35	557.60	0.00	36	557.60	2.00
37	590.40	0.00	38	590.40	2.00	39	623.20	0.00

40 623.20 2.00 41 656.00 0.00 42 656.00 2.00

BOUNDARY CONDITION DATA

NUMBER OF STEADY DIRICHLET NODES (NBTO) = 0
NUMBER OF STEADY FLUX NODES (NDFLUX) = 0
NUMBER OF TRANSIENT DIRICHLET NODES (NBHVAR) = 0
NUMBER OF TRANSIENT FLUX NODES (NBFVAR) = 0

NUMBER OF DECAYING SOURCE BOUNDARY NODES(NDCS) = 2

DECAYING SOURCE DATA

SOURCE IDENTIFICATION NUMBER 1

LEACH TIME DURATION = 0.100E+07
DECAY COEFFICIENT FOR SPECIES COMPONENT 1 = 0.160E-02
DECAY COEFFICIENT FOR SPECIES COMPONENT 2 = 0.462E-01
DECAY COEFFICIENT FOR SPECIES COMPONENT 3 = 0.106E-03

SOURCE NODE BOUNDARY CONDITIONS

NODE NUMBER = 1 SOURCE I.D. NUMBER = 1
BOUNDARY CONDITION INDEX = 2 NET FLUID FLUX = 0.239E+03
LIST OF PRESCRIBED SOLUTE MASS FLUX FOR COMPONENTS 1 TO NSPECI

0.239E+03 0.000E+00 0.000E+00

NODE NUMBER = 2 SOURCE I.D. NUMBER = 1
BOUNDARY CONDITION INDEX = 2 NET FLUID FLUX = 0.239E+03
LIST OF PRESCRIBED SOLUTE MASS FLUX FOR COMPONENTS 1 TO NSPECI

0.239E+03 0.000E+00 0.000E+00

DEFAULT VALUES AND WEIGHTING FACTORS

DEFAULT VALUE OF X-VELOCITY(VCX) = 0.2394E+03
DEFAULT VALUE OF Y-VELOCITY(VCY) = 0.0000E+00
X-DIRECTION UPSTREAM WEIGHTING FACTOR(WFAC) = 0.1000E+00
Y-DIRECTION UPSTREAM WEIGHTING FACTOR(YFAC) = 0.0000E+00
DEFAULT WATER SATURATION(SWD) = 0.1000E+01
STEADY-STATE VELOCITY FIELD (0=NO, 1=YES).(IVSTED) = 1

LIST OF BOUNDARY NODE NUMBERS:

1 2 41 42

BOUNDARY NODAL DATA

 NODE FLUID FLOW RATE
 ---- -
 1 239.4
 2 239.4
 41 -239.4
 42 -239.4

----- ACTUAL HALF BAND WIDTH = 3 FULL BANDWIDTH = 7 -----

*** ELEMENT CENTROIDAL COORDINATES ***

ELEMENT	X-COOR.	Y-COOR.	ELEMENT	X-COOR.	Y-COOR.	ELEMENT	X-COOR.	Y-COOR.
1	16.40	1.00	2	49.20	1.00	3	82.00	1.00
4	114.80	1.00	5	147.60	1.00	6	180.40	1.00
7	213.20	1.00	8	246.00	1.00	9	278.80	1.00
10	311.60	1.00	11	344.40	1.00	12	377.20	1.00
13	410.00	1.00	14	442.80	1.00	15	475.60	1.00
16	508.40	1.00	17	541.20	1.00	18	574.00	1.00
19	606.80	1.00	20	639.60	1.00			

LIST OF OBSERVATION NODES

19 19 19

LIST OF SELECTED DEPENDENT VARIABLES

1 2 3

+++++++ BEGIN TRANSIENT CALCULATIONS +++++++

**** ELAPSED SIMULATION TIME : 18.20 TIME STEP NUMBER : 1 TIME STEP SIZE: 0.182E+02 ****

**** ELAPSED SIMULATION TIME : 36.40 TIME STEP NUMBER : 2 TIME STEP SIZE: 0.182E+02 ****

**** ELAPSED SIMULATION TIME : 54.60 TIME STEP NUMBER : 3 TIME STEP SIZE: 0.182E+02 ****

*** NODAL DISPERSIVE FLUX VALUES ***

NODE	DISP. FLUX	NODE	DISP. FLUX	NODE	DISP. FLUX	NODE	DISP. FLUX	NODE	DISP. FLUX
1	69.29	2	69.29	41	-3.3448E-27	42	3.4079E-28		

.....
SUM OF ABOVE FLUX VALUES = 138.58
.....

SPECIES COMPONENT NUMBER 1
.....

*** INCREMENTAL MASS BALANCE RESULTS OVER A TIME STEP ***
.....

TOTAL DISPERSIVE FLUX RATE	138.58
TOTAL ADVECTIVE FLUX RATE	271.67
TOTAL DISPERSIVE + ADVECTIVE FLUX RATE	410.25
RATE OF MASS DECAY AND TRANSFORMATION	29.932
NET RATE OF MATERIAL ACCUMULATION	410.25
MASS BALANCE ERROR	-8.09648E-06
NORMALIZED MASS BALANCE ERROR	9.86778E-09
RATE OF MASS ACCUMULATION DUE TO PRESSURE HEAD CHANGE	0.00000E+00

*** CUMULATIVE MASS BALANCE RESULTS ***
.....

CUMULATIVE MATERIAL STORAGE	22168.
CUMULATIVE MASS DECAY AND TRANSFORMATION	1126.0

*** NODAL DISPERSIVE FLUX VALUES ***
.....

NODE	DISP. FLUX	NODE	DISP. FLUX	NODE	DISP. FLUX	NODE	DISP. FLUX	NODE	DISP. FLUX
1	2.164	2	2.164	41	-1.8302E-28	42	-1.1991E-28		

.....
SUM OF ABOVE FLUX VALUES = 4.3288
.....

SPECIES COMPONENT NUMBER 2
.....

*** INCREMENTAL MASS BALANCE RESULTS OVER A TIME STEP ***
.....

TOTAL DISPERSIVE FLUX RATE	4.3288
TOTAL ADVECTIVE FLUX RATE	8.7375
TOTAL DISPERSIVE + ADVECTIVE FLUX RATE	13.066
RATE OF MASS DECAY AND TRANSFORMATION	-1.7753
NET RATE OF MATERIAL ACCUMULATION	13.066
MASS BALANCE ERROR	-2.60398E-07
NORMALIZED MASS BALANCE ERROR	9.96448E-09
RATE OF MASS ACCUMULATION DUE TO PRESSURE HEAD CHANGE	0.00000E+00

*** CUMULATIVE MASS BALANCE RESULTS ***
.....

CUMULATIVE MATERIAL STORAGE	744.51
CUMULATIVE MASS DECAY AND TRANSFORMATION.....	-134.36

*** NODAL DISPERSIVE FLUX VALUES ***

NODE	DISP. FLUX	NODE	DISP. FLUX	NODE	DISP. FLUX	NODE	DISP. FLUX	NODE	DISP. FLUX
1	2.794	2	2.794	41	-5.6798E-29	42	-9.4663E-30		

SUM OF ABOVE FLUX VALUES = 5.5885

SPECIES COMPONENT NUMBER 3

*** INCREMENTAL MASS BALANCE RESULTS OVER A TIME STEP ***

TOTAL DISPERSIVE FLUX RATE	5.5885
TOTAL ADVECTIVE FLUX RATE	15.092
TOTAL DISPERSIVE + ADVECTIVE FLUX RATE	20.680
RATE OF MASS DECAY AND TRANSFORMATION	-28.030
NET RATE OF MATERIAL ACCUMULATION	20.680
MASS BALANCE ERROR	-4.49770E-07
NORMALIZED MASS BALANCE ERROR	1.08744E-08
RATE OF MASS ACCUMULATION DUE TO PRESSURE HEAD CHANGE	0.00000E+00

*** CUMULATIVE MASS BALANCE RESULTS ***

CUMULATIVE MATERIAL STORAGE	1641.6
CUMULATIVE MASS DECAY AND TRANSFORMATION.....	-987.83

*** NODAL CONCENTRATIONS FOR SPECIES NO. 1 ***

1	0.6269	2	0.6269	3	6.0830E-02	4	6.0830E-02	5	-1.4873E-02
6	-1.4873E-02	7	1.6366E-03	8	1.6366E-03	9	-2.2165E-05	10	-2.2165E-05
11	-4.4453E-05	12	-4.4453E-05	13	1.5614E-05	14	1.5614E-05	15	-3.9366E-06
16	-3.9366E-06	17	8.6847E-07	18	8.6847E-07	19	-1.7821E-07	20	-1.7821E-07
21	3.4944E-08	22	3.4944E-08	23	-6.6428E-09	24	-6.6428E-09	25	1.2347E-09
26	1.2347E-09	27	-2.2562E-10	28	-2.2562E-10	29	4.0681E-11	30	4.0681E-11
31	-7.2572E-12	32	-7.2572E-12	33	1.2833E-12	34	1.2833E-12	35	-2.2527E-13
36	-2.2527E-13	37	3.9361E-14	38	3.9361E-14	39	-7.0742E-15	40	-7.0742E-15
41	2.1461E-15	42	2.1461E-15						

*** NODAL CONCENTRATIONS FOR SPECIES NO. 2 ***

1	2.0953E-02	2	2.0953E-02	3	2.0814E-03	4	2.0814E-03	5	-4.8238E-04
6	-4.8238E-04	7	4.9374E-05	8	4.9374E-05	9	-7.8981E-08	10	-7.8981E-08
11	-1.3800E-06	12	-1.3800E-06	13	4.2992E-07	14	4.2992E-07	15	-9.6016E-08
16	-9.6016E-08	17	1.8151E-08	18	1.8151E-08	19	-3.0025E-09	20	-3.0025E-09
21	4.2237E-10	22	4.2237E-10	23	-4.2964E-11	24	-4.2964E-11	25	-2.1599E-13

26	-2.1599E-13	27	1.8120E-12	28	1.8120E-12	29	-7.0478E-13	30	-7.0478E-13
31	2.0549E-13	32	2.0549E-13	33	-5.3014E-14	34	-5.3014E-14	35	1.2769E-14
36	1.2769E-14	37	-2.9496E-15	38	-2.9496E-15	39	6.9060E-16	40	6.9060E-16
41	-2.7135E-16	42	-2.7135E-16						

*** NODAL CONCENTRATIONS FOR SPECIES NO. 3 ***

1	4.1864E-02	2	4.1864E-02	3	6.4503E-03	4	6.4503E-03	5	-6.4655E-04
6	-6.4655E-04	7	-1.5383E-05	8	-1.5383E-05	9	1.5222E-05	10	1.5222E-05
11	-3.0512E-06	12	-3.0512E-06	13	3.8105E-07	14	3.8105E-07	15	-1.7148E-08
16	-1.7148E-08	17	-7.5997E-09	18	-7.5997E-09	19	3.2696E-09	20	3.2696E-09
21	-8.9447E-10	22	-8.9447E-10	23	2.0571E-10	24	2.0571E-10	25	-4.2754E-11
26	-4.2754E-11	27	8.2534E-12	28	8.2534E-12	29	-1.4942E-12	30	-1.4942E-12
31	2.5322E-13	32	2.5322E-13	33	-3.9542E-14	34	-3.9542E-14	35	5.4440E-15
36	5.4440E-15	37	-5.7050E-16	38	-5.7050E-16	39	4.1120E-18	40	4.1120E-18
41	4.1042E-17	42	4.1042E-17						

**** ELAPSED SIMULATION TIME : 72.80 TIME STEP NUMBER : 4 TIME STEP SIZE: 0.182E+02 ****

**** ELAPSED SIMULATION TIME : 91.00 TIME STEP NUMBER : 5 TIME STEP SIZE: 0.182E+02 ****

**** ELAPSED SIMULATION TIME : 109.2 TIME STEP NUMBER : 6 TIME STEP SIZE: 0.182E+02 ****

*** NODAL DISPERSIVE FLUX VALUES ***

NODE	DISP. FLUX	NODE	DISP. FLUX	NODE	DISP. FLUX	NODE	DISP. FLUX	NODE	DISP. FLUX
1	21.38	2	21.38	41	-3.8774E-26	42	2.1326E-25		

SUM OF ABOVE FLUX VALUES = 42.769

SPECIES COMPONENT NUMBER 1

*** INCREMENTAL MASS BALANCE RESULTS OVER A TIME STEP ***

TOTAL DISPERSIVE FLUX RATE	42.769
TOTAL ADVECTIVE FLUX RATE	355.24
TOTAL DISPERSIVE + ADVECTIVE FLUX RATE	398.01
RATE OF MASS DECAY AND TRANSFORMATION	61.406
NET RATE OF MATERIAL ACCUMULATION	398.01
MASS BALANCE ERROR	-1.05870E-05
NORMALIZED MASS BALANCE ERROR	1.32999E-08
RATE OF MASS ACCUMULATION DUE TO PRESSURE HEAD CHANGE	0.00000E+00

*** CUMULATIVE MASS BALANCE RESULTS ***

CUMULATIVE MATERIAL STORAGE	41442.
CUMULATIVE MASS DECAY AND TRANSFORMATION.....	3921.5

*** NODAL DISPERSIVE FLUX VALUES ***

NODE	DISP. FLUX	NODE	DISP. FLUX	NODE	DISP. FLUX	NODE	DISP. FLUX	NODE	DISP. FLUX
1	0.7527	2	0.7527	41	-3.3321E-27	42	-1.0097E-28		

SUM OF ABOVE FLUX VALUES = 1.5054

SPECIES COMPONENT NUMBER 2

*** INCREMENTAL MASS BALANCE RESULTS OVER A TIME STEP ***

TOTAL DISPERSIVE FLUX RATE	1.5054
TOTAL ADVECTIVE FLUX RATE	12.614
TOTAL DISPERSIVE + ADVECTIVE FLUX RATE	14.120
RATE OF MASS DECAY AND TRANSFORMATION	1.6015
NET RATE OF MATERIAL ACCUMULATION	14.120
MASS BALANCE ERROR	-3.75940E-07
NORMALIZED MASS BALANCE ERROR	1.33124E-08
RATE OF MASS ACCUMULATION DUE TO PRESSURE HEAD CHANGE	0.00000E+00

*** CUMULATIVE MASS BALANCE RESULTS ***

CUMULATIVE MATERIAL STORAGE	1477.7
CUMULATIVE MASS DECAY AND TRANSFORMATION.....	-99.309

*** NODAL DISPERSIVE FLUX VALUES ***

NODE	DISP. FLUX	NODE	DISP. FLUX	NODE	DISP. FLUX	NODE	DISP. FLUX	NODE	DISP. FLUX
1	2.560	2	2.560	41	1.6156E-27	42	-4.0390E-28		

SUM OF ABOVE FLUX VALUES = 5.1200

.....

SPECIES COMPONENT NUMBER 3

*** INCREMENTAL MASS BALANCE RESULTS OVER A TIME STEP ***

TOTAL DISPERSIVE FLUX RATE	5.1200
TOTAL ADVECTIVE FLUX RATE	50.673
TOTAL DISPERSIVE + ADVECTIVE FLUX RATE	55.793
RATE OF MASS DECAY AND TRANSFORMATION	-62.396
NET RATE OF MATERIAL ACCUMULATION	55.793
MASS BALANCE ERROR	-1.51017E-06
NORMALIZED MASS BALANCE ERROR	1.35337E-08
RATE OF MASS ACCUMULATION DUE TO PRESSURE HEAD CHANGE	0.00000E+00

*** CUMULATIVE MASS BALANCE RESULTS ***

CUMULATIVE MATERIAL STORAGE	6843.6
CUMULATIVE MASS DECAY AND TRANSFORMATION.....	-3795.5

*** NODAL CONCENTRATIONS FOR SPECIES NO. 1 ***

1	0.7504	2	0.7504	3	0.2866	4	0.2866	5	2.0662E-02
6	2.0662E-02	7	-8.2668E-03	8	-8.2668E-03	9	5.0555E-04	10	5.0555E-04
11	1.9317E-04	12	1.9317E-04	13	-6.9308E-05	14	-6.9308E-05	15	1.2228E-05
16	1.2228E-05	17	-9.0301E-07	18	-9.0301E-07	19	-2.4135E-07	20	-2.4135E-07
21	1.2893E-07	22	1.2893E-07	23	-3.7031E-08	24	-3.7031E-08	25	8.1614E-09
26	8.1614E-09	27	-1.4422E-09	28	-1.4422E-09	29	1.8364E-10	30	1.8364E-10
31	-4.1055E-12	32	-4.1055E-12	33	-7.5247E-12	34	-7.5247E-12	35	3.4219E-12
36	3.4219E-12	37	-1.0979E-12	38	-1.0979E-12	39	3.2005E-13	40	3.2005E-13
41	-1.4733E-13	42	-1.4733E-13						

*** NODAL CONCENTRATIONS FOR SPECIES NO. 2 ***

1	2.6748E-02	2	2.6748E-02	3	1.0223E-02	4	1.0223E-02	5	7.3800E-04
6	7.3800E-04	7	-2.9405E-04	8	-2.9405E-04	9	1.7888E-05	10	1.7888E-05
11	6.8481E-06	12	6.8481E-06	13	-2.4459E-06	14	-2.4459E-06	15	4.2973E-07
16	4.2973E-07	17	-3.1676E-08	18	-3.1676E-08	19	-8.3287E-09	20	-8.3287E-09
21	4.4280E-09	22	4.4280E-09	23	-1.2617E-09	24	-1.2617E-09	25	2.7572E-10
26	2.7572E-10	27	-4.8416E-11	28	-4.8416E-11	29	6.2225E-12	30	6.2225E-12
31	-2.1572E-13	32	-2.1572E-13	33	-2.0621E-13	34	-2.0621E-13	35	9.4531E-14
36	9.4531E-14	37	-2.9269E-14	38	-2.9269E-14	39	8.0261E-15	40	8.0261E-15
41	-3.3738E-15	42	-3.3738E-15						

*** NODAL CONCENTRATIONS FOR SPECIES NO. 3 ***

1	0.1191	2	0.1191	3	4.8140E-02	4	4.8140E-02	5	4.8961E-03
6	4.8961E-03	7	-1.1546E-03	8	-1.1546E-03	9	2.8246E-07	10	2.8246E-07
11	3.5474E-05	12	3.5474E-05	13	-8.0486E-06	14	-8.0486E-06	15	8.4437E-07
16	8.4437E-07	17	5.4419E-08	18	5.4419E-08	19	-4.8650E-08	20	-4.8650E-08
21	1.3521E-08	22	1.3521E-08	23	-2.5910E-09	24	-2.5910E-09	25	3.4938E-10
26	3.4938E-10	27	-1.8224E-11	28	-1.8224E-11	29	-7.6437E-12	30	-7.6437E-12
31	3.4970E-12	32	3.4970E-12	33	-9.6092E-13	34	-9.6092E-13	35	2.0875E-13
36	2.0875E-13	37	-3.7166E-14	38	-3.7166E-14	39	4.9526E-15	40	4.9526E-15
41	-1.1641E-16	42	-1.1641E-16						

**** ELAPSED SIMULATION TIME : 127.4 TIME STEP NUMBER : 7 TIME STEP SIZE: 0.182E+02 ****

**** ELAPSED SIMULATION TIME : 145.6 TIME STEP NUMBER : 8 TIME STEP SIZE: 0.182E+02 ****

**** ELAPSED SIMULATION TIME : 163.8 TIME STEP NUMBER : 9 TIME STEP SIZE: 0.182E+02 ****

*** NODAL DISPERSIVE FLUX VALUES ***

NODE	DISP. FLUX	NODE	DISP. FLUX	NODE	DISP. FLUX	NODE	DISP. FLUX	NODE	DISP. FLUX
1	7.201	2	7.201	41	1.8095E-25	42	-7.7548E-26		

SUM OF ABOVE FLUX VALUES = 14.402

SPECIES COMPONENT NUMBER 1

*** INCREMENTAL MASS BALANCE RESULTS OVER A TIME STEP ***

TOTAL DISPERSIVE FLUX RATE	14.402
TOTAL ADVECTIVE FLUX RATE	356.41
TOTAL DISPERSIVE + ADVECTIVE FLUX RATE	370.81
RATE OF MASS DECAY AND TRANSFORMATION	88.447
NET RATE OF MATERIAL ACCUMULATION	370.81
MASS BALANCE ERROR	-1.06218E-05
NORMALIZED MASS BALANCE ERROR	1.43224E-08
RATE OF MASS ACCUMULATION DUE TO PRESSURE HEAD CHANGE	0.00000E+00

*** CUMULATIVE MASS BALANCE RESULTS ***

CUMULATIVE MATERIAL STORAGE	57849.
CUMULATIVE MASS DECAY AND TRANSFORMATION	8277.8

*** NODAL DISPERSIVE FLUX VALUES ***

NODE	DISP. FLUX	NODE	DISP. FLUX	NODE	DISP. FLUX	NODE	DISP. FLUX	NODE	DISP. FLUX
1	0.2575	2	0.2575	41	-8.0779E-27	42	4.8468E-27		

SUM OF ABOVE FLUX VALUES = 0.51501

SPECIES COMPONENT NUMBER 2

*** INCREMENTAL MASS BALANCE RESULTS OVER A TIME STEP ***

TOTAL DISPERSIVE FLUX RATE	0.51501
TOTAL ADVECTIVE FLUX RATE	12.774
TOTAL DISPERSIVE + ADVECTIVE FLUX RATE	13.289
RATE OF MASS DECAY AND TRANSFORMATION	3.0956
NET RATE OF MATERIAL ACCUMULATION	13.289
MASS BALANCE ERROR	-3.80701E-07
NORMALIZED MASS BALANCE ERROR	1.43237E-08
RATE OF MASS ACCUMULATION DUE TO PRESSURE HEAD CHANGE	0.00000E+00

*** CUMULATIVE MASS BALANCE RESULTS ***

CUMULATIVE MATERIAL STORAGE	2074.2
CUMULATIVE MASS DECAY AND TRANSFORMATION	46.992

*** NODAL DISPERSIVE FLUX VALUES ***

NODE	DISP. FLUX	NODE	DISP. FLUX	NODE	DISP. FLUX	NODE	DISP. FLUX	NODE	DISP. FLUX
1	1.527	2	1.527	41	3.3927E-26	42	-1.2925E-26		

SUM OF ABOVE FLUX VALUES = 3.0546

SPECIES COMPONENT NUMBER 3

*** INCREMENTAL MASS BALANCE RESULTS OVER A TIME STEP ***

TOTAL DISPERSIVE FLUX RATE	3.0546
TOTAL ADVECTIVE FLUX RATE	87.491
TOTAL DISPERSIVE + ADVECTIVE FLUX RATE	90.545
RATE OF MASS DECAY AND TRANSFORMATION	-90.063
NET RATE OF MATERIAL ACCUMULATION	90.545
MASS BALANCE ERROR	-2.60743E-06
NORMALIZED MASS BALANCE ERROR	1.43985E-08
RATE OF MASS ACCUMULATION DUE TO PRESSURE HEAD CHANGE	0.00000E+00

*** CUMULATIVE MASS BALANCE RESULTS ***

CUMULATIVE MATERIAL STORAGE 15604.
CUMULATIVE MASS DECAY AND TRANSFORMATION..... -8234.5

*** NODAL CONCENTRATIONS FOR SPECIES NO. 1 ***

1	0.7394	2	0.7394	3	0.4437	4	0.4437	5	0.1284
6	0.1284	7	4.1898E-03	8	4.1898E-03	9	-4.2579E-03	10	-4.2579E-03
11	2.4212E-04	12	2.4212E-04	13	1.3485E-04	14	1.3485E-04	15	-3.8490E-05
16	-3.8490E-05	17	3.3965E-06	18	3.3965E-06	19	8.5592E-07	20	8.5592E-07
21	-4.2145E-07	22	-4.2145E-07	23	9.4078E-08	24	9.4078E-08	25	-1.0959E-08
26	-1.0959E-08	27	-8.8262E-10	28	-8.8262E-10	29	8.8953E-10	30	8.8953E-10
31	-2.9188E-10	32	-2.9188E-10	33	6.6951E-11	34	6.6951E-11	35	-1.1184E-11
36	-1.1184E-11	37	9.5299E-13	38	9.5299E-13	39	2.4525E-13	40	2.4525E-13
41	-2.9101E-13	42	-2.9101E-13						

*** NODAL CONCENTRATIONS FOR SPECIES NO. 2 ***

1	2.6509E-02	2	2.6509E-02	3	1.5909E-02	4	1.5909E-02	5	4.6038E-03
6	4.6038E-03	7	1.5025E-04	8	1.5025E-04	9	-1.5264E-04	10	-1.5264E-04
11	8.6782E-06	12	8.6782E-06	13	4.8319E-06	14	4.8319E-06	15	-1.3789E-06
16	-1.3789E-06	17	1.2170E-07	18	1.2170E-07	19	3.0618E-08	20	3.0618E-08
21	-1.5077E-08	22	-1.5077E-08	23	3.3653E-09	24	3.3653E-09	25	-3.9242E-10
26	-3.9242E-10	27	-3.1222E-11	28	-3.1222E-11	29	3.1655E-11	30	3.1655E-11
31	-1.0388E-11	32	-1.0388E-11	33	2.3829E-12	34	2.3829E-12	35	-3.9877E-13
36	-3.9877E-13	37	3.4526E-14	38	3.4526E-14	39	8.3836E-15	40	8.3836E-15
41	-1.0100E-14	42	-1.0100E-14						

*** NODAL CONCENTRATIONS FOR SPECIES NO. 3 ***

1	0.1950	2	0.1950	3	0.1193	4	0.1193	5	3.6253E-02
6	3.6253E-02	7	2.0587E-03	8	2.0587E-03	9	-1.0729E-03	10	-1.0729E-03
11	1.5172E-05	12	1.5172E-05	13	3.7608E-05	14	3.7608E-05	15	-7.8096E-06
16	-7.8096E-06	17	2.4567E-07	18	2.4567E-07	19	2.6780E-07	20	2.6780E-07
21	-8.6456E-08	22	-8.6456E-08	23	1.4265E-08	24	1.4265E-08	25	-6.4641E-10
26	-6.4641E-10	27	-4.3794E-10	28	-4.3794E-10	29	1.8098E-10	30	1.8098E-10
31	-4.3811E-11	32	-4.3811E-11	33	7.4304E-12	34	7.4304E-12	35	-6.8909E-13
36	-6.8909E-13	37	-9.2992E-14	38	-9.2992E-14	39	7.3106E-14	40	7.3106E-14
41	-4.2143E-14	42	-4.2143E-14						

**** ELAPSED SIMULATION TIME : 182.0 TIME STEP NUMBER : 10 TIME STEP SIZE: 0.182E+02 ****

**** ELAPSED SIMULATION TIME : 200.2 TIME STEP NUMBER : 11 TIME STEP SIZE: 0.182E+02 ****

**** ELAPSED SIMULATION TIME : 218.4 TIME STEP NUMBER : 12 TIME STEP SIZE: 0.182E+02 ****

*** NODAL DISPERSIVE FLUX VALUES ***

NODE	DISP. FLUX	NODE	DISP. FLUX	NODE	DISP. FLUX	NODE	DISP. FLUX	NODE	DISP. FLUX
1	2.659	2	2.659	41	-4.3944E-25	42	-3.6189E-25		

SUM OF ABOVE FLUX VALUES = 5.3174

SPECIES COMPONENT NUMBER 1

*** INCREMENTAL MASS BALANCE RESULTS OVER A TIME STEP ***

TOTAL DISPERSIVE FLUX RATE	5.3174
TOTAL ADVECTIVE FLUX RATE	336.25
TOTAL DISPERSIVE + ADVECTIVE FLUX RATE	341.57
RATE OF MASS DECAY AND TRANSFORMATION	110.83
NET RATE OF MATERIAL ACCUMULATION	341.57
MASS BALANCE ERROR	-1.00211E-05
NORMALIZED MASS BALANCE ERROR	1.46692E-08
RATE OF MASS ACCUMULATION DUE TO PRESSURE HEAD CHANGE	0.00000E+00

*** CUMULATIVE MASS BALANCE RESULTS ***

CUMULATIVE MATERIAL STORAGE	71367.
CUMULATIVE MASS DECAY AND TRANSFORMATION	13940.

*** NODAL DISPERSIVE FLUX VALUES ***

NODE	DISP. FLUX	NODE	DISP. FLUX	NODE	DISP. FLUX	NODE	DISP. FLUX	NODE	DISP. FLUX
1	9.5322E-02	2	9.5322E-02	41	3.5543E-26	42	-2.2618E-26		

SUM OF ABOVE FLUX VALUES = 0.19064

SPECIES COMPONENT NUMBER 2

*** INCREMENTAL MASS BALANCE RESULTS OVER A TIME STEP ***

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TOTAL DISPERSIVE FLUX RATE ..... 0.19064
TOTAL ADVECTIVE FLUX RATE ..... 12.062
TOTAL DISPERSIVE + ADVECTIVE FLUX RATE ..... 12.253
RATE OF MASS DECAY AND TRANSFORMATION ..... 3.9676
NET RATE OF MATERIAL ACCUMULATION ..... 12.253
MASS BALANCE ERROR ..... -3.59473E-07
NORMALIZED MASS BALANCE ERROR ..... 1.46693E-08
RATE OF MASS ACCUMULATION DUE TO PRESSURE HEAD CHANGE ..... 0.00000E+00
  
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*** CUMULATIVE MASS BALANCE RESULTS ***

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CUMULATIVE MATERIAL STORAGE ..... 2560.1
CUMULATIVE MASS DECAY AND TRANSFORMATION..... 248.97
  
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*** NODAL DISPERSIVE FLUX VALUES ***

NODE	DISP. FLUX	NODE	DISP. FLUX	NODE	DISP. FLUX	NODE	DISP. FLUX	NODE	DISP. FLUX
1	0.8418	2	0.8418	41	-3.0050E-25	42	-1.5510E-25		

SUM OF ABOVE FLUX VALUES = 1.6836

SPECIES COMPONENT NUMBER 3

*** INCREMENTAL MASS BALANCE RESULTS OVER A TIME STEP ***

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TOTAL DISPERSIVE FLUX RATE ..... 1.6836
TOTAL ADVECTIVE FLUX RATE ..... 120.75
TOTAL DISPERSIVE + ADVECTIVE FLUX RATE ..... 122.44
RATE OF MASS DECAY AND TRANSFORMATION ..... -112.11
NET RATE OF MATERIAL ACCUMULATION ..... 122.44
MASS BALANCE ERROR ..... -3.59878E-06
NORMALIZED MASS BALANCE ERROR ..... 1.46963E-08
RATE OF MASS ACCUMULATION DUE TO PRESSURE HEAD CHANGE ..... 0.00000E+00
  
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*** CUMULATIVE MASS BALANCE RESULTS ***

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CUMULATIVE MATERIAL STORAGE ..... 27462.
CUMULATIVE MASS DECAY AND TRANSFORMATION..... -13975.
  
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*** NODAL CONCENTRATIONS FOR SPECIES NO. 1 ***

1	0.6940	2	0.6940	3	0.5198	4	0.5198	5	0.2435
6	0.2435	7	5.4710E-02	8	5.4710E-02	9	-9.5934E-04	10	-9.5934E-04
11	-2.0936E-03	12	-2.0936E-03	13	1.6324E-04	14	1.6324E-04	15	7.2110E-05

16	7.2110E-05	17	-1.9642E-05	18	-1.9642E-05	19	6.5202E-07	20	6.5202E-07
21	8.0163E-07	22	8.0163E-07	23	-2.4530E-07	24	-2.4530E-07	25	2.9886E-08
26	2.9886E-08	27	3.4836E-09	28	3.4836E-09	29	-2.6901E-09	30	-2.6901E-09
31	7.2488E-10	32	7.2488E-10	33	-1.1042E-10	34	-1.1042E-10	35	8.6488E-13
36	8.6488E-13	37	5.7104E-12	38	5.7104E-12	39	-2.3278E-12	40	-2.3278E-12
41	9.8365E-13	42	9.8365E-13						

*** NODAL CONCENTRATIONS FOR SPECIES NO. 2 ***

1	2.4895E-02	2	2.4895E-02	3	1.8648E-02	4	1.8648E-02	5	8.7346E-03
6	8.7346E-03	7	1.9626E-03	8	1.9626E-03	9	-3.4414E-05	10	-3.4414E-05
11	-7.5103E-05	12	-7.5103E-05	13	5.8559E-06	14	5.8559E-06	15	2.5866E-06
16	2.5866E-06	17	-7.0455E-07	18	-7.0455E-07	19	2.3394E-08	20	2.3394E-08
21	2.8751E-08	22	2.8751E-08	23	-8.7983E-09	24	-8.7983E-09	25	1.0720E-09
26	1.0720E-09	27	1.2487E-10	28	1.2487E-10	29	-9.6456E-11	30	-9.6456E-11
31	2.5993E-11	32	2.5993E-11	33	-3.9605E-12	34	-3.9605E-12	35	3.1609E-14
36	3.1609E-14	37	2.0453E-13	38	2.0453E-13	39	-8.3402E-14	40	-8.3402E-14
41	3.5255E-14	42	3.5255E-14						

*** NODAL CONCENTRATIONS FOR SPECIES NO. 3 ***

1	0.2631	2	0.2631	3	0.1989	4	0.1989	5	9.4871E-02
6	9.4871E-02	7	2.2464E-02	8	2.2464E-02	9	1.6058E-04	10	1.6058E-04
11	-7.9218E-04	12	-7.9218E-04	13	3.2938E-05	14	3.2938E-05	15	2.8890E-05
16	2.8890E-05	17	-5.9692E-06	18	-5.9692E-06	19	-1.1397E-07	20	-1.1397E-07
21	2.9811E-07	22	2.9811E-07	23	-7.0039E-08	24	-7.0039E-08	25	5.0831E-09
26	5.0831E-09	27	1.8834E-09	28	1.8834E-09	29	-8.3015E-10	30	-8.3015E-10
31	1.7534E-10	32	1.7534E-10	33	-1.7495E-11	34	-1.7495E-11	35	-2.7349E-12
36	-2.7349E-12	37	1.8586E-12	38	1.8586E-12	39	-5.5487E-13	40	-5.5487E-13
41	1.7767E-13	42	1.7767E-13						

**** ELAPSED SIMULATION TIME : 236.6 TIME STEP NUMBER : 13 TIME STEP SIZE: 0.182E+02 ****

**** ELAPSED SIMULATION TIME : 254.8 TIME STEP NUMBER : 14 TIME STEP SIZE: 0.182E+02 ****

**** ELAPSED SIMULATION TIME : 273.0 TIME STEP NUMBER : 15 TIME STEP SIZE: 0.182E+02 ****

*** NODAL DISPERSIVE FLUX VALUES ***

NODE	DISP. FLUX	NODE	DISP. FLUX	NODE	DISP. FLUX	NODE	DISP. FLUX	NODE	DISP. FLUX
1	1.067	2	1.067	41	1.6770E-24	42	8.1749E-25		

SUM OF ABOVE FLUX VALUES = 2.1345

SPECIES COMPONENT NUMBER 1

*** INCREMENTAL MASS BALANCE RESULTS OVER A TIME STEP ***

TOTAL DISPERSIVE FLUX RATE	2.1345
TOTAL ADVECTIVE FLUX RATE	311.42
TOTAL DISPERSIVE + ADVECTIVE FLUX RATE	313.56
RATE OF MASS DECAY AND TRANSFORMATION	128.93
NET RATE OF MATERIAL ACCUMULATION	313.56
MASS BALANCE ERROR	-9.28108E-06
NORMALIZED MASS BALANCE ERROR	1.47997E-08
RATE OF MASS ACCUMULATION DUE TO PRESSURE HEAD CHANGE	0.00000E+00

*** CUMULATIVE MASS BALANCE RESULTS ***

CUMULATIVE MATERIAL STORAGE	82263.
CUMULATIVE MASS DECAY AND TRANSFORMATION.....	20666.

*** NODAL DISPERSIVE FLUX VALUES ***

NODE	DISP. FLUX	NODE	DISP. FLUX	NODE	DISP. FLUX	NODE	DISP. FLUX	NODE	DISP. FLUX
1	3.8282E-02	2	3.8282E-02	41	9.0473E-26	42	-6.4623E-26		

SUM OF ABOVE FLUX VALUES = 7.65637E-02

SPECIES COMPONENT NUMBER 2

*** INCREMENTAL MASS BALANCE RESULTS OVER A TIME STEP ***

TOTAL DISPERSIVE FLUX RATE	7.65637E-02
TOTAL ADVECTIVE FLUX RATE	11.172
TOTAL DISPERSIVE + ADVECTIVE FLUX RATE	11.249
RATE OF MASS DECAY AND TRANSFORMATION	4.6246
NET RATE OF MATERIAL ACCUMULATION	11.249
MASS BALANCE ERROR	-3.32951E-07
NORMALIZED MASS BALANCE ERROR	1.47997E-08
RATE OF MASS ACCUMULATION DUE TO PRESSURE HEAD CHANGE	0.00000E+00

*** CUMULATIVE MASS BALANCE RESULTS ***

CUMULATIVE MATERIAL STORAGE 2951.1
CUMULATIVE MASS DECAY AND TRANSFORMATION..... 490.16

*** NODAL DISPERSIVE FLUX VALUES ***

NODE	DISP. FLUX	NODE	DISP. FLUX	NODE	DISP. FLUX	NODE	DISP. FLUX	NODE	DISP. FLUX
1	0.4629	2	0.4629	41	5.5576E-25	42	6.3331E-25		

SUM OF ABOVE FLUX VALUES = 0.92587

SPECIES COMPONENT NUMBER 3

*** INCREMENTAL MASS BALANCE RESULTS OVER A TIME STEP ***

TOTAL DISPERSIVE FLUX RATE 0.92587
TOTAL ADVECTIVE FLUX RATE 150.49
TOTAL DISPERSIVE + ADVECTIVE FLUX RATE 151.41
RATE OF MASS DECAY AND TRANSFORMATION -129.38
NET RATE OF MATERIAL ACCUMULATION 151.41
MASS BALANCE ERROR -4.48491E-06
NORMALIZED MASS BALANCE ERROR 1.48101E-08
RATE OF MASS ACCUMULATION DUE TO PRESSURE HEAD CHANGE 0.00000E+00

*** CUMULATIVE MASS BALANCE RESULTS ***

CUMULATIVE MATERIAL STORAGE 41981.
CUMULATIVE MASS DECAY AND TRANSFORMATION..... -20743.

*** NODAL CONCENTRATIONS FOR SPECIES NO. 1 ***

1	0.6416	2	0.6416	3	0.5422	4	0.5422	5	0.3316
6	0.3316	7	0.1261	8	0.1261	9	2.1639E-02	10	2.1639E-02
11	-1.8670E-03	12	-1.8670E-03	13	-9.7054E-04	14	-9.7054E-04	15	1.1414E-04
16	1.1414E-04	17	3.4490E-05	18	3.4490E-05	19	-1.0172E-05	20	-1.0172E-05
21	8.3446E-08	22	8.3446E-08	23	4.9422E-07	24	4.9422E-07	25	-1.1980E-07
26	-1.1980E-07	27	5.0528E-09	28	5.0528E-09	29	4.9210E-09	30	4.9210E-09
31	-1.7190E-09	32	-1.7190E-09	33	2.6743E-10	34	2.6743E-10	35	6.9921E-12
36	6.9921E-12	37	-1.7058E-11	38	-1.7058E-11	39	5.6787E-12	40	5.6787E-12
41	-1.6421E-12	42	-1.6421E-12						

*** NODAL CONCENTRATIONS FOR SPECIES NO. 2 ***

1	2.3018E-02	2	2.3018E-02	3	1.9452E-02	4	1.9452E-02	5	1.1895E-02
6	1.1895E-02	7	4.5221E-03	8	4.5221E-03	9	7.7628E-04	10	7.7628E-04

11	-6.6976E-05	12	-6.6976E-05	13	-3.4817E-05	14	-3.4817E-05	15	4.0945E-06
16	4.0945E-06	17	1.2373E-06	18	1.2373E-06	19	-3.6492E-07	20	-3.6492E-07
21	2.9940E-09	22	2.9940E-09	23	1.7729E-08	24	1.7729E-08	25	-4.2977E-09
26	-4.2977E-09	27	1.8127E-10	28	1.8127E-10	29	1.7653E-10	30	1.7653E-10
31	-6.1666E-11	32	-6.1666E-11	33	9.5937E-12	34	9.5937E-12	35	2.5071E-13
36	2.5071E-13	37	-6.1189E-13	38	-6.1189E-13	39	2.0371E-13	40	2.0371E-13
41	-5.8909E-14	42	-5.8909E-14						

*** NODAL CONCENTRATIONS FOR SPECIES NO. 3 ***

1	0.3241	2	0.3241	3	0.2751	4	0.2751	5	0.1697
6	0.1697	7	6.5811E-02	8	6.5811E-02	9	1.2058E-02	10	1.2058E-02
11	-6.7317E-04	12	-6.7317E-04	13	-5.0581E-04	14	-5.0581E-04	15	4.1079E-05
16	4.1079E-05	17	1.8792E-05	18	1.8792E-05	19	-4.2795E-06	20	-4.2795E-06
21	-1.6628E-07	22	-1.6628E-07	23	2.3720E-07	24	2.3720E-07	25	-4.5106E-08
26	-4.5106E-08	27	-5.7306E-10	28	-5.7306E-10	29	2.4100E-09	30	2.4100E-09
31	-6.5523E-10	32	-6.5523E-10	33	7.2781E-11	34	7.2781E-11	35	1.1027E-11
36	1.1027E-11	37	-7.3609E-12	38	-7.3609E-12	39	1.9182E-12	40	1.9182E-12
41	-3.8686E-13	42	-3.8686E-13						

*** OBSERVATION NODE INFORMATION ***

NODAL VALUES OF DEPENDENT VARIABLE OVER TIME

OBSERVED NODE NUMBER: 19 SPECIES COMPONENT NUMBER : 1

TIME	CONCENTRATION	TIME	CONCENTRATION	TIME	CONCENTRATION	TIME	CONCENTRATION
0.1820E+02	0.3111E+00	0.3640E+02	0.5079E+00	0.5460E+02	0.6269E+00	0.7280E+02	0.6962E+00
0.9100E+02	0.7335E+00	0.1092E+03	0.7504E+00	0.1274E+03	0.7541E+00	0.1456E+03	0.7494E+00
0.1638E+03	0.7394E+00	0.1820E+03	0.7260E+00	0.2002E+03	0.7106E+00	0.2184E+03	0.6940E+00
0.2366E+03	0.6767E+00	0.2548E+03	0.6592E+00	0.2730E+03	0.6416E+00		

OBSERVED NODE NUMBER: 19 SPECIES COMPONENT NUMBER : 2

TIME	CONCENTRATION	TIME	CONCENTRATION	TIME	CONCENTRATION	TIME	CONCENTRATION
0.1820E+02	0.7921E-02	0.3640E+02	0.1554E-01	0.5460E+02	0.2095E-01	0.7280E+02	0.2420E-01
0.9100E+02	0.2594E-01	0.1092E+03	0.2675E-01	0.1274E+03	0.2698E-01	0.1456E+03	0.2685E-01
0.1638E+03	0.2651E-01	0.1820E+03	0.2604E-01	0.2002E+03	0.2549E-01	0.2184E+03	0.2489E-01
0.2366E+03	0.2428E-01	0.2548E+03	0.2365E-01	0.2730E+03	0.2302E-01		

OBSERVED NODE NUMBER: 19 SPECIES COMPONENT NUMBER : 3

TIME	CONCENTRATION	TIME	CONCENTRATION	TIME	CONCENTRATION	TIME	CONCENTRATION
0.1820E+02	0.7293E-03	0.3640E+02	0.1976E-02	0.5460E+02	0.6450E-02	0.7280E+02	0.1568E-01
0.9100E+02	0.2979E-01	0.1092E+03	0.4814E-01	0.1274E+03	0.6979E-01	0.1456E+03	0.9380E-01
0.1638E+03	0.1193E+00	0.1820E+03	0.1457E+00	0.2002E+03	0.1723E+00	0.2184E+03	0.1989E+00
0.2366E+03	0.2250E+00	0.2548E+03	0.2504E+00	0.2730E+03	0.2751E+00		

***** VAM2D HAS FULLY EXECUTED *****

11 REFERENCES

- Abeelee, W.V., M.L. Wheeler, and B.W. Burton, 1981. Geohydrology of Bandelier Tuff, Report No. LA-8962-MS, Los Alamos National Lab., Los Alamos, New Mexico, 50 pp.
- Anderson, M.P., and H.F. Wang, 1982. Introduction to Groundwater Modeling. Freeman and Co., San Francisco.
- Bear, J., 1979. Hydraulics of Groundwater, McGraw-Hill, New York.
- Bear, J. and A. Verruijt, 1987. Modeling Groundwater Flow and Pollution. D. Reidel Publishing Company, Norwell, MA.
- Brooks, R.H., and A.T. Corey, 1966. Properties of porous media affecting fluid flow, ASCE J. Irrig. Drain. Div., 92(IR2):61-88.
- Carsel, R.F. et al., 1985. The pesticide root zone model (PRZM), Ecological Modeling, 30:46-69.
- Coats, K.H., and B.D. Smith, 1964. Dead-end pore volume and dispersion in porous media, Soc. of Petrol. Engrs. J., 4, 4, pp. 73-83.
- Cooley, R.L., 1983. Some new procedures for numerical solution of variably saturated flow problems, Water Resour. Res., v. 19, no. 5, pp. 1271-1285.
- Davis, L.A., and S.P. Neuman, December, 1983. Documentation and User's Guide: UNSAT2-Variably Saturated Flow Model, U.S. Nuclear Regulatory Commission, NUREG/CR-3390, Washington, D.C.
- de Marsily, G., 1986. Quantitative Hydrogeology, Academic Press, Inc., Orlando, Florida.
- Duguid, J., and M. Reeves, 1976. Material transport in porous media: A finite element Galerkin model, Rep. ORNL-4928, Oak Ridge National Lab., Oak Ridge, Tennessee.
- Enfield, C.G. et al., 1983. Methods for approximating pollutant transport to groundwater, Ground Water, 20:711-722.
- Feddes, R.A., E. Bresler, and S.P. Neuman 1974. Field test of a modified numerical model for water uptake by root systems, Water Resour. Res., v. 10, no. 6, pp. 1199-1206.

- Frind, E.O., R.W. Gillham, and J.F. Pickens, 1977. Application of unsaturated flow properties in the design of geologic environments for radioactive waste storage facilities, *Finite Elements in Water Resources*, edited by W.G. Gray, G.F. Pinder, and C.A. Brebbia, Pentech Press, Plymouth, England, pp. 3.133-3.163.
- Gillham, R.W., A. Klute, and D.F. Heermann, 1979. Measurement and numerical simulation of hysteretic flow in a heterogeneous porous medium, *Soil Sci. Soc. Am. J.*, v. 43, pp. 1061-1067.
- Hanks, R.J., A. Klute, and E. Bresler, 1969. A numeric method for estimating infiltration, redistribution, drainage, and evaporation of water from soil, *Water Resour. Res.*, v. 5, no. 5, pp. 1064-1069.
- Huyakorn, P.S., and K. Nilkuha, 1979. Solution of transient transport equation using an upstream finite element scheme, *Applied Mathematical Model.*, v. 3, pp. 7-17.
- Huyakorn, P.S., and G.F. Pinder, 1983. Computational Methods in Subsurface Flow, Academic Press, Orlando, Florida, 474 pp.
- Huyakorn, P.S., B.G. Jones, J.C. Parker, T.D. Wadsworth, and H.O. White, Jr., April, 1987. "Finite element simulation of moisture movement and solute transport in a large caisson", in *Modeling Study of Solute Transport in the Unsaturated Zone: Workshop Proceedings*, NUREG/CR-4615, vol. 2, U.S. Nuclear Regulatory Commission, pp. 117-170.
- Huyakorn, P.S., T.D. Wadsworth, H.O. White, Jr., and J.E. Buckley, 1987. VADOFT Version 3.2: Finite element code for simulating one-dimensional flow and solute transport in the vadose zone, Project Report, prepared by HydroGeoLogic, Inc. for U.S. EPA Environmental Research Lab., Athens, Georgia.
- Huyakorn, P.S., J.W. Mercer, and D.S. Ward, 1985. Finite element matrix and mass balance computational schemes for transport in variably saturated porous media, *Water Resour. Res.*, v. 21, no. 3, pp. 346-358.
- Huyakorn, P.S., S.D. Thomas, and B.M. Thompson, 1984. Techniques for making finite elements competitive in modeling flow in variably saturated porous media, *Water Resour. Res.*, v. 20, no. 8, pp. 1099-1115.
- Istok, J., 1989. Groundwater Modeling by the Finite Element Method. Water Resources Monograph No. 13, American Geophysical Union, Washington, D.C.
- Kalf, F.R.P., 1988. A variably saturated finite element model for three-dimensional seepage face problems, Ph.D. Thesis, the Univ. of New South Wales, Sydney, Australia, 339 pp.

- Kool, J.B., and J.C. Parker, 1987. Development and evaluation of closed-form expressions for hysteretic soil hydraulic properties, *Water Resour. Res.*, v. 23, pp. 105-114.
- McCord, J.T., D.B. Stephens, and J.L. Wilson, 1988. Field experiments and numerical simulations of unsaturated flow and transport: The roles of hysteresis and state-dependent anisotropy. *Proc. Nato Advanced Study Institute on Recent Advances in Modeling Hydrologic Systems*, Sintra, Portugal, July 9-23.
- Millington, R.J. and J.M. Quirk, 1961. Permeability of Porous Solids. *Trans. Faraday Society*, 57:1200-1207.
- Montaglou, A., and L.W. Gelhar, 1987. Effective hydraulic conductivities of transient unsaturated flow in stratified soils, *Water Resour. Res.*, v. 23, pp. 57-68.
- Mualem, Y., 1976. A new model for predicting the hydraulic conductivity of unsaturated porous media, *Water Resour. Res.*, v. 12, no. 3, pp. 513-522.
- Neuman, S.P., R.A. Feddes, and E. Bresler, 1974. Finite element simulation of flow in saturated-unsaturated soils considering water uptake by plants, *Hydrodynamics and Hydraulic Engineering Laboratory Report for Project No. ALO-SWC-77*, Haifa, Israel.
- Nyhan, J., W. Polzer, E. Essington, E. Cokal, L. Lane, E. Lopez, E. Stallings, and R. Walker, 1986. A joint DOE/NRC field study of tracer migration in the unsaturated zone, Los Alamos National Lab., Report no. LA-10575-MS, 201 pp.
- Perlmutter, N.M., and M. Lieber, 1970. Dispersion of plating wastes and sewage contaminants in groundwater and surface water, South Farmingdale-Massapequa Area, Nassau County, New York, U.S. Geol. Surv. Water Supply Paper 1879-G.
- Reeves, M., and R.M. Cranwell, April, 1981. User's manual for the Sandia-waste isolation flow and transport model (SWIFT) 4-81, NUREG/CR-2324, U.S. Nuclear Regulatory Commission, 145 pp.
- Robertson, J.B., 1984. Geologic Problems at Low-Level Radioactive Waste Sites, in: Groundwater Contamination, National Research Council, National Academy Press, pp. 104-109.
- Rubin, J., 1968. Theoretical analysis of two-dimensional transient flow of water in unsaturated and partly unsaturated soils, *Soil Sci. Soc. Am. Proc.*, v. 32, no. 5, pp. 607-615.
- Scheidegger, A.E., 1961. General theory of dispersion in porous media, *J. Geophys. Res.*, v. 66, pp. 3273-3278.

- Silka, L.R., and J.W. Mercer, 1982. Evaluation of remedial actions for groundwater contamination at Love Canal, New York, presented at the National Conference on Management of Uncontrolled Hazardous Wastes Sites, Hazardous Mater. Contr. Res. Inst., Silver Spring, Maryland.
- Sudicky, E.A., 1989. The Laplace Transform Galerkin technique: A time-continuous finite element theory and application to mass transport in groundwater, *Water Resour. Res.*, v.25, pp. 1833-1846.
- van Genuchten, M.Th., J.C. Parker, and J.B. Kool, April, 1987. "Analysis and prediction of water and solute transport in a large lysimeter", in *Modeling Study of Solute Transport in the Unsaturated Zone: Workshop Proceedings*, NUREG/CR-4615, vol. 2, U.S. Nuclear Regulatory Commission, pp. 4-31.
- van Genuchten, M.Th., G.F. Pinder, and W.P. Saukin, 1977. Modeling of leachate and soil interactions in an aquifer, *Management of Gas and Leachate in Landfills*, U.S. Environmental Protection Agency, Rep. EPA-600/9-77-026, pp. 95-103.
- van Genuchten, M.Th., 1980. A closed-form equation for predicting the hydraulic conductivity of unsaturated soils. *Soil Science Soc. of Am. Journal* 44:892-898.
- Wilson, J.L., and P.J. Miller, 1978. Two-dimensional plume in uniform ground-water flow, *J. of the Hydraulics Div., Amer. Soc. Civ. Engrs.* 104, HY4, 1978.
- Yeh, G.T., and D.S. Ward, 1981, FEMWASTE: A finite-element model of waste transport through saturated-unsaturated porous media, Rep. ORNL-5601, Oak Ridge National Lab., Oak Ridge, Tennessee, 137 pp.
- Yeh, T.-C. J., L.W. Gelhar, and A.L. Gutjahr, 1985. Stochastic analysis of unsaturated flow in heterogeneous soils 2. Statistically anisotropic media with variable α , *Water Resour. Res.*, v. 21, pp. 457-464.