Auxiliary Analyses in Support of Performance Assessment of a Hypothetical Low-Level Waste Facility

Two-Phase Flow and Contaminant Transport in Unsaturated
Soils with Application to Low-Level Radioactive Waste Disposal

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Abstract

A numerical model of multiphase air-water flow and contaminant transport in the unsaturated zone is presented. The multiphase flow equations are solved using the two-pressure, mixed form of the equations with a modified Picard linearization of the equations and a finite element spatial approximation. A volatile contaminant is assumed to be transported in either phase, or in both phases simultaneously. The contaminant partitions between phases with an equilibrium distribution given by Henry's Law or via kinetic mass transfer. The transport equations are solved using a Galerkin finite element method with reduced integration to lump the resultant matrices. The numerical model is applied to published experimental studies to examine the behavior of the air phase and associated contaminant movement under water infiltration. The model is also used to evaluate a hypothetical design for a low-level radioactive waste disposal facility. The model has been developed in both one and two dimensions; documentation and computer codes are available for the one-dimensional flow and transport model.

Contents

<i>Abstract</i>	<i>iii</i>
<i>Contents</i>	<i>v</i>
<i>Figures, List of</i>	<i>vii</i>
<i>Tables, List of</i>	<i>ix</i>
<i>Executive Summary</i>	<i>xi</i>
<i>Foreword</i>	<i>xiii</i>
<i>Acknowledgments</i>	<i>xv</i>
<i>Introduction</i>	<i>1</i>
1. Governing equations	3
Flow equations	3
Darcy's Law	4
Constitutive relations	5
Two-pressure equation formulation	8
Transport equations	9
Governing equations	9
Contaminant partitioning	12
Sorption	12
Vapor-liquid equilibria	13
Equilibrium mass transfer	13
Non-equilibrium partitioning	13
Discussion	14
References	15
2. Numerical solution of two-pressure equations	19
Introduction	19
Numerical solution in one dimension	21
Temporal discretization: Modified Picard iteration scheme	22
Spatial discretization: Galerkin finite element scheme	23
Temporal lumping	27
Boundary conditions	28
Mass balance	29
Calculation of mass flux	30
Numerical results in one dimension	30
Verification of numerical scheme	30
Air phase velocities	31
Example 1. Open column, 8.3 cm/h flux rate	34

Example 2. Bounded column, 8.3cm/h flux	34
Example 3. Bounded column, 20cm/h flux	36
Numerical properties and comparison to head-based formulation	36
Two-dimensional numerical solution	36
Time lumping	42
Source/Sink terms	43
Boundary conditions	43
Air equation	43
Verification of code and example problems	44
Discussion	52
References	52
 3. <i>Solution of the transport equations by finite elements</i>	 57
Introduction	57
Equation formulation: Equilibrium case	59
One-dimensional finite element solution	60
Numerical behavior of the solution	63
Lumping	63
Time weighting	64
Kinetic mass transfer in one dimension	64
Transport in water phase only	66
Equilibrium partitioning	66
Kinetic mass transfer	66
Two-dimensional contaminant transport	71
Lumping in space by numerical integration	71
Mass balance	72
Example simulations	73
Gas phase migration from designed LLW containment facilities	73
Design of LLW disposal facilities	73
Biologic methane production	73
Application of the two-phase air and water flow and contaminant transport model to the facility design	79
Vapor phase diffusion through the layered system	79
Vapor-phase migration to the perimeter of the vault	81
Source term	81
Assumptions	84
Results of the model	84
Discussion	90
References	90
 <i>Closing Remarks</i>	 95
References	95
 <i>Appendix</i>	 A-1

Figures, List of

Figure 1-1	Capillary pressure and relative permeability as functions of saturation for the experimental data of Touma and Vauclin (1986).	7
Figure 1-2	Effective molecular diffusion coefficient vs. Saturation of air, a comparison of formulations.	11
Figure 2-1	Basis functions for the one-dimensional finite element solution of the flow equation.	25
Figure 2-2	Experimental setup for Example 3 of Table 2-1 showing boundary conditions before and after ponding occurs. Darker shading indicates higher water content.	32
Figure 2-3	Time evolution of moisture content profile comparing the numerical results with those of Touma and Vauclin (1986). (Note that the results of Touma and Vauclin depicted here are an approximate representation of the figure in their paper).	33
Figure 2-4	Time evolution of infiltrating water front (as shown in gray scale) and air movement (shown as particle trajectories) for Example 1: open column with a flux rate of 8.3 cmh^{-1} applied to the surface.	35
Figure 2-5	Time evolution of air and water pressures (profiles plotted at 10 min intervals) for Example 2: bounded column with a flux rate of 8.3 cmh^{-1} applied to the surface.	37
Figure 2-6	Time evolution of infiltrating water front (as shown in gray scale) and air movement (shown as particle trajectories) for Example 3: bounded column with a flux rate of 20 cmh^{-1} applied to the surface.	38
Figure 2-7	Mass balance for air and water as a function of time, using the mixed form of the equations and using the head-based form of the equations.	39
Figure 2-8	Boundary conditions for the comparison of the one-dimensional and two-dimensional two-phase flow codes.	45
Figure 2-9	Comparison of one- and two-dimensional two-phase flow codes for the boundary and initial conditions illustrated in Figure 2-8 and different discretization sizes.	46
Figure 2-10	Material distribution, boundary and initial conditions for infiltration from a strip source into a uniform initially dry transect of coarse Touma and Vauclin (1986) sand.	47
Figure 2-11	Flow solution for infiltration into a uniform coarse Touma and Vauclin (1986) sand. The figure shows the water infiltration in gray scale and has superposed the paths of particles of air.	48
Figure 2-12	Pressure-saturation curves for the coarse sand of Touma and Vauclin (1986) and a hypothetical loam.	49
Figure 2-13	Material distribution, boundary and initial conditions for infiltration from a strip source into a transect of coarse Touma and Vauclin (1986) sand embedded with loam lenses. The numbering of the lenses is used in the discussion in the text.	50
Figure 2-14	Flow solution for infiltration into a coarse Touma and Vauclin (1986) sand embedded with loam lenses at time 25 hours.	51
Figure 3-1	Flow of air and water in a 100 cm column with a water flux of 20 cm/h at the surface. Water content at a given time in the column is shown in gray scale by a vertical slice through the diagram. Air particle paths are delineated by the lines on the diagram.	65
Figure 3-2	Contaminant transport only in the water phase. Concentration profiles with depth are shown at 10 minute intervals.	67
Figure 3-3	TCE contaminant plume evolution in time with equilibrium partitioning between the water and air phases.	68
Figure 3-4	Concentration in the water phase with a kinetic mass transfer between the water and air phases.	69

Figure 3-5	Air concentration for kinetic mass transfer of pollutants with $c_w=1$ initially in the water phase at 30-35 cm depth.	70
Figure 3-6	Domain for model problem.	72
Figure 3-7	Analytical solution for contaminant transport from a strip source of length 1cm at the top left of the domain.	74
Figure 3-8	Lumped finite element solution of the problem illustrated in Figure 3-7.	75
Figure 3-9	Contaminant transport solution for infiltration into a homogeneous material using the velocities of water obtained from the solution shown in Figure 2-11.	76
Figure 3-10	Multilayered capillary barrier system over the containment cells.	77
Figure 3-11	Subsurface concrete cell drainage system.	78
Figure 3-12	Layered system used in the one - dimensional simulations.	80
Figure 3-13	Cross-section of vault layers to be modeled in two dimensions.	82
Figure 3-14	Discretization and boundary conditions for two-dimensional simulation.	83
Figure 3-15	Case 1 moisture content contours and air particle movement vectors at 3 months.	85
Figure 3-16	Case 1 concentration profiles; (a) time = 3 months, (b) time = 3 years, (c) time = 8 years.	86
Figure 3-17	Case 2 moisture content contours and air particle movement vectors at 3 months.	87
Figure 3-18	Case 2 concentration profiles; (a) time = 3 months, (b) time = 3 years, (c) time = 8 years.	88
Figure 3-19	Case 3 concentration profiles; (a) time = 5 years, (b) time = 20 years, (c) time = 100 years.	89

Tables, List of

Table 2-1	Boundary conditions for the experiments of Touma and Vauclin (1986).	31
Table 3-1	Summary of available vapor-phase flow and transport models.	58
Table 3-2	Summary of formulation differences for the effective molecular diffusion coefficient.	81
Table 3-3	Van Genuchten parameters in layered system model.	81

Executive Summary

A comprehensive description of contaminant transport in unsaturated soils requires inclusion of transport processes in both the water and air phases, as well as mass transfer between phases (including the solid phase) and any reactions that occur within each phase. Because transport in the water phase may be quite different from transport in the air phase, analysis of possible exposure pathways should include dynamic transport in both fluid phases. A numerical simulator that predicts fluid flow and contaminant transport in the air and water phases, with both equilibrium and kinetic mass transfer between phases, has been developed to study problems of contaminant transport in unsaturated soils. The simulator is based on an extension of numerical methods developed previously for Richards' equation. These numerical methods are robust and mass-conservative. Example simulations demonstrate the dynamic response of the air phase to different infiltration scenarios in one- and two-dimensional porous media. Long-term gas migration from a hypothetical design facility is also included as an example calculation.

When solving two-phase porous media flow equations, the coupled, nonlinear nature of the governing equations generally requires use of numerical solution methods. The numerical methods developed in this work are based on a modified Picard linearization of a lumped finite element approximation. The modified Picard approach assures numerical mass balance, while the lumping procedure controls nonphysical oscillations in the solution. Lumping is accomplished via numerical integration using the trapezoid rule. Application of the simulator demonstrates the dynamic response of the air phase under infiltration conditions. In particular, the simulation results demonstrate that significant air flows occur, independent of the applicability of Richards' equation, and that significant fluxes of air from the soil to the atmosphere should be expected during early times for almost all infiltration events. Whether or not this outgassing from the soil is important to contaminant transport depends on the volatilization characteristics of the contaminant. Equilibrium partitioning based on the appropriate Henry's constant leads to enhanced spatial mixing because of the different phase velocities for the water and air flows. Kinetic partitioning can lead to significantly different results, relative to equilibrium partitioning. This can lead to significantly more contaminant outgassing than is predicted by the equilibrium results. This can be important if short-time results associated with individual infiltration events are analyzed. Hydraulic and capillary data for most of the one-dimensional simulations were taken from laboratory experiments reported in the literature, while contaminant partitioning data were taken from standard tabulated values and from specific laboratory measurements. The code was validated by comparison to measurements of infiltration in laboratory columns. Documentation for the one-dimensional code is included as the Appendix; the complete computer code is available through the Energy Science and Technology Software Center, P.O. Box 1020, Oak Ridge, TN 378310.

The one-dimensional simulations were based on short-term laboratory experiments. While longer-term processes can be investigated with a one-dimensional simulator, practical analyses of longer-term contaminant migration may require multi-dimensional simulators. To examine more general transport systems, a two-dimensional version of the simulator has been developed. This code was tested against one-dimensional results and against simple two-dimensional solutions. The code was used to examine a few scenarios involving material heterogeneities and their influence on multiphase flow systems. It was also used to examine gas-phase transport of volatile radioactive components generated at a hypothetical low-level radioactive waste disposal facility. An interesting aspect of the problem is the hypothetical design of the drain system within the concrete vaults that hold the waste. The drain, designed to prevent any water that might breach the container from accumulating within the vault, provides a direct pathway for gas-phase migration of any volatile contaminants in the vault. Therefore, the production rate of contaminants within the vault acts as a forcing function for the air phase in the porous media surrounding the vaults. This means that the designed vaults provide no containment for gas-phase contaminants. Assuming a layered capillary-barrier system above the vault system, with high moisture content in the clay layers, low diffusion through those layers acts to direct the contaminants to the lateral boundaries of the capillary barrier system. Depending on the source term within the vault, travel-time estimates for contaminants to reach the lateral boundary of the capillary barrier system are on the order of ten to one hundred years. Once the contaminants reach the lateral boundary of the capillary barrier system, detailed estimates of surface fluxes could be obtained using one-dimensional simulations.

Foreword

This technical report was prepared by Princeton University under a subcontract to Massachusetts Institute of Technology as part of their research project with the Waste Management Branch in the Office of Nuclear Regulatory Research (FIN D2044). The report presents a numerical model for multiphase air-water flow and contaminant transport in the unsaturated zone. The report also presents simulations using the documented multiphase model for a hypothetical low-level radioactive waste (LLW) disposal design and inventory. This work is the second volume in a series (NUREG/CR-6114) of contractors' reports which provide auxiliary analysis in support of the NRC staff development and testing of a performance assessment methodology for LLW facilities. This document provides technical discussion of issues arising from multiphase flow and contaminant transport analyses using a proposed engineering design, and hypothetical site conditions and processes relevant to LLW disposal.

Volume 2 of NUREG/CR-6114 is not a substitute for NRC regulations, and compliance is not required. The approaches and/or methods described in this NUREG/CR are provided for information only. Publication of this report does not necessarily constitute NRC approval or agreement with the information contained herein.

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Introduction

Unsaturated-zone processes are important in many branches of science and engineering. These include soil science, agricultural science, hydrology, and hydrogeology. One of the prominent features of the unsaturated zone is that it provides the link between the atmosphere and the deeper subsurface. Fluid exchange at the land surface provides important hydrologic and atmospheric connections. Both water and air are exchanged at the land surface, so the behavior of both air and water in the unsaturated zone must be understood.

Historically, air movement in the unsaturated zone has not been considered to be important. In the fields of soil science and hydrology, the focus of most problems has been water movement. Because the air is much less viscous than water, it usually does not build up pressure much above atmospheric pressure. Therefore, Richards' assumption that the air remains at constant atmospheric pressure is often a good assumption, and Richards' equation is adequate to describe the movement of water in unsaturated soils. The fact that air often remains at essentially atmospheric pressure has been used by many authors in the literature to claim that the air phase is stagnant. This incorrect logic leads to an erroneous picture of the unsaturated zone. The correct statement is that despite the lack of significant air-pressure changes, the air phase is highly mobile and has volumetric fluxes that are essentially equal in magnitude to the volumetric fluxes of water.

The movement of air in the unsaturated zone can be important to understand the transport and fate of various volatile contaminants. Therefore air-phase dynamics may be important to problems involving non-aqueous-phase liquid (NAPL) spills in the unsaturated zone, to problems associated with leaky tanks or pipelines, and to problems that involve waste disposal in unsaturated soils, including low-level radioactive waste disposal sites. To study the possible importance of coupled water- and air-phase dynamics, with associated contaminant transport in each phase and contaminant transfer between phases, a general two-phase model was developed. This model solves the coupled set of partial differential equations that describes water and air movement in the unsaturated zone. A second set of partial differential equations, describing the movement of contaminants dissolved in, and partitioned between, the two fluid phases, is then solved. This numerical model allows a wide range of problems to be studied, including model problems that can demonstrate fundamental features of unsaturated systems.

The numerical model is based on a finite element solution to the equations, with certain refinements to the general finite element approach. These include the use of a Modified Picard linearization in the flow solution, and reduced integration procedures in the transport equation to control spatial oscillations that can occur in multi-dimensional problems. The model allows for time-varying boundary conditions and fully heterogeneous material properties. Contaminant partitioning can be either equilibrium (Henry's Law) or kinetic. Documentation for the one-dimensional version of this code is provided as Appendix A of this document.

The presentation herein begins with a section describing the governing equation for both the fluid flow and contaminant transport processes. Salient features of these equations include fully nonlinear descriptions of the flow equation parameters, general kinetic partitioning, and a nonlinear effective diffusion coefficient (as a function of moisture content) for the air phase. The next section, section 2, outlines the numerical procedure used in the fluid flow solution. The method used is the lumped finite element method, with a Modified Picard procedure used for linearization. Example problems are solved to demonstrate the dynamic nature of the air phase under natural infiltration events. Out-gassing at the land surface is shown to be an expected behavior for soils during infiltration. Both one-dimensional and two-dimensional problems show this behavior. Two-dimensional simulations in heterogeneous media are presented to demonstrate the abilities of the model to effectively handle natural heterogeneities.

Section 3 describes the numerical methods used to solve the contaminant transport equations. Example calculations are used to demonstrate the potential importance of contaminant partitioning behavior in the overall movement of volatile contaminants. A second example problem involves a suite of simulations examining a particular engineering design for possible use in low-level radioactive waste disposal. Several general points are raised by this analysis. First, a design focused on control of water can (and in this case, does) provide direct pathways for contaminant movement in the air phase out of containment structures to the surrounding porous media. Once in the porous media, the air-phase transport is controlled in large part by the source term (that is, gas production rate) within the containment cell. Long-term integrity of the engineered barriers is also an important consideration. Finally, the simulations demonstrate that short-term versus long-term time scales involve significantly different assumptions, with concomitant differences in the resulting mathematical descriptions of the systems.

The final section presents general concluding remarks. This is followed by an appendix in which documentation of the one-dimensional version of the unsaturated-zone simulator is presented. The associated software is available from the Energy Science and Technology Software Center, P.O. Box 1020, Oak Ridge, TN 378310.

1. Governing equations

The equations that describe fluid flow and contaminant transport in the unsaturated zone will be reviewed in this section. The two-phase flow equations will be presented in what will be called the two - pressure form (standard mass balance form) that is commonly used by hydrologists. In addition, the transport equations will be given for each phase and the mass transfer processes between phases will be discussed.

Several assumptions are made in the equations presented. The most important of which are listed here. Others will be mentioned in the body of the section.

- There are assumed to be three phases present in the system: a solid, liquid and gas phase. The solid phase is assumed to be immobile and consolidated. The gas and liquid phases are assumed to be fully mobile, but are assumed to be immiscible.
- The media is assumed to be isothermal. Heat is an important variable in mass transfer between phases but is neglected here.
- The flow of the two fluids is independent of the presence of contaminant in either phase. This assumption allows the solution of the flow equation independently of the transport equation. In some situations that will not be considered here, the density of the air will be dependent upon the vapor phase concentration of contaminant.

1-1. Flow equations

The unsaturated zone is, by definition, a multiphase system, because at least two fluid phases are present: air and water. A macroscopic description of this system uses solid and fluid properties defined over the porous media continuum, and is based on conservation laws applied to each fluid phase present. These balance laws are then augmented by material-dependent constitutive relationships; in the unsaturated zone, the main relationships are the capillary pressure - saturation relation and the relative permeability - saturation relation. The combination of mass balance equations and appropriate constitutive equations results in a set of governing equations for the multi-phase unsaturated-zone system.

In this work the unsaturated zone will be considered as a multiphase system and equations will be written for both the air and water phases. In most previous work on the unsaturated zone the air-phase equation is eliminated by the assumption that the air-phase remains essentially at atmospheric pressure. This assumption is reasonable in most cases because the mobility of the air phase is much larger than that of water, due to the viscosity difference between the two fluids. This assumption does not imply that the air phase is stagnant but rather just the opposite, namely that the air phase has a very high mobility. When the air-phase pressure is assumed constant and equal to atmospheric pressure, the air-phase mass balance equation is eliminated and only one phase equation remains. Further assumptions of constant water density and negligible porosity changes lead to the Richards equation (Hillel 1980, Morel-Seytoux 1973).

Richards equation is usually adequate to represent the movement of water in unsaturated soils. However, it provides no information on the motion of the air phase. If contaminant transport is the main concern, and the contaminant can be transported in the vapor phase, then it is unlikely that the use of Richards equation is justifiable *a priori* (see Celia and Binning 1992a). While the air phase may have insignificant effects on the motion of the water phase, it may still need to be included to determine the advective component of air-phase contaminant transport. In such cases the coupled set of nonlinear equations that describe air and water motion in the unsaturated zone need to be solved.

The mass balance equation for each of the fluid phases can be written [Bear (1979)].

$$\frac{\partial (\phi \rho_{\alpha} \theta_{\alpha})}{\partial t} + \nabla \cdot (\rho_{\alpha} q_{\alpha}) = F_{\alpha} \quad (\text{Eq. 1-1})$$

with the following notation:

α	subscript denoting the phase to which the equation applies. In this work α will refer to air and water unless otherwise noted.
ϕ	porosity [L^3/L^3]
ρ_{α}	density of phase α [M/L^3]
S_{α}	Saturation of phase α [L^3/L^3]
q_{α}	Volumetric flux (or Darcy flux) of phase α [$L/[T]$]

1-2. Darcy's Law

$$F_{\alpha} \quad \text{Source or sink of fluid } \alpha \text{ [M][L]}^{-3}[\text{T}]^{-1}$$

This equation can be written in many ways with different dependant variables and constitutive relations. Two of the ways of writing this equation are the two-pressure approach and the pressure-saturation formulation of the equations, as discussed in detail by Binning (1994). In this work, the two-pressure approach will be used.

It is useful to introduce the concept of a volumetric fluid content of phase α , which is defined by:

$$\theta_{\alpha} = \phi S_{\alpha} \quad (\text{Eq. 1-2})$$

When the volumetric fluid content is used the flow equation (Eq. 1-1) becomes:

$$\frac{\partial (\rho_{\alpha} \theta_{\alpha})}{\partial t} + \nabla \cdot (\rho_{\alpha} \mathbf{q}) = F_{\alpha} \quad (\text{Eq. 1-3})$$

1-2. Darcy's Law

Darcy's Law relates volumetric flux of a fluid phase to the pressure of that phase. This equation may be viewed as a statement of momentum balance (Dullien, 1979; Gray and Hassanizadeh, 1991), or as an empirically-derived constitutive relationship. The generalized multiphase Darcy's Law may be written as:

$$\mathbf{q}_{\alpha} = -\frac{k k_{r\alpha}}{\mu_{\alpha}} (\nabla p_{\alpha} - \rho_{\alpha} \mathbf{g}) \quad (\text{Eq. 1-4})$$

where:

- k is the intrinsic permeability tensor of the medium $[\text{L}]^2$
- $k_{r\alpha}$ is the relative permeability of phase α $[\text{L}]^0$
- μ_{α} is the dynamic viscosity of fluid α $[\text{M}][\text{L}]^{-1}[\text{T}]^{-1}$
- p_{α} is the fluid pressure of phase α $[\text{M}][\text{L}]^{-1}[\text{T}]^{-2}$
- $\mathbf{g}$ is the acceleration due to gravity vector $[\text{L}][\text{T}]^{-2}$

The multiphase version of Darcy's Law introduces the relative permeability function, which is typically a nonlinear function of fluid saturation. It ranges in value from 0 when the fluid is not present (or present at saturation below residual) to 1 when the fluid occupies all of the pores (saturation of 1).

Darcy's Law is a linear relation between the gradient of fluid pressure and the fluid flux. It is valid for viscous dominated flow which occurs at low velocities. At higher fluid velocities, slip flow, or non zero flux along the pore walls is increasingly important and Darcy's law must be modified to include additional terms. Massman (1989) discussed the validity of Darcy's law during soil venting experiments. He concludes that Darcy's law is a good approximation for air flow in sands and gravels and a fair approximation in materials with smaller pores such as silts, clays and other low permeability materials. In this work, Darcy's Law is assumed to be valid for both the water and air phases.

In the disciplines of hydrology and soil science it is very common to replace the definition of pressure in (Eq. 1-4) with the pressure in equivalent water column height. This is called the pressure head and is defined by:

$$h_{\alpha} = \frac{p_{\alpha}}{\rho_{ow} g}$$

At times it is also useful to introduce the non-linear conductivity tensor K which is related to the permeability by:

$$K_{\alpha} = \frac{\rho_{ow} g k k_{r\alpha}}{\mu_{\alpha}} = K_{\alpha} k_{r\alpha} \quad (\text{Eq. 1-5})$$

where:

- ρ_{ow} density of water at standard temperature and pressure $[\text{M}]/[\text{L}]^3$
- g the magnitude of the acceleration due to gravity $[\text{L}]/[\text{T}]^2$
- K_{α} the conductivity when the porous medium is saturated with fluid α

Using these definitions Darcy's law can be written equivalently as:

$$q_{\alpha} = -K_{\alpha} \left(\nabla h_{\alpha} - \frac{\rho_{\alpha}}{\rho_{ow}} i_z \right) \quad (\text{Eq. 1-6})$$

with i_z the unit normal oriented downwards in the direction of the force of gravity. Note that this work adopts the convention common in soil science and hydrology of orienting the z axis downward. This convention is adopted so that infiltration flux at the surface has a positive sign.

The volumetric flux can be thought of as the volume of fluid α passing through a unit area of porous medium per unit time. When we wish to follow the path of a contaminant in the flow field described by (Eq. 1-1), it is necessary to describe the average flow velocity, rather than the volumetric flux. The flow velocity $[L][T]^{-1}$ is defined as:

$$v_{\alpha} = \frac{q_{\alpha}}{\theta_{\alpha}} \quad (\text{Eq. 1-7})$$

1-3. Constitutive relations

Equations (Eq. 1-3) and (Eq. 1-4) describe the flow conditions in the system. There are several unknowns in these equations. In order to close the system constitutive relations that relate the unknowns must be specified. These constitutive relations can be written in a variety of ways that result in different variables becoming the independent variables for the system. The most common choices for independent variables are the individual phase pressures and the phase saturations.

In this section three constitutive relations will be specified. They are the pressure-saturation, relative permeability-saturation, and density-pressure relations.

The fluid saturation is a function of the difference between the pressure of the two fluids in the porous medium. The pressure difference is called the capillary pressures and it is defined as:

$$p_c \equiv p_a - p_w$$

with corresponding definition for the capillary pressure head:

$$h_c \equiv h_a - h_w$$

Many different functional forms have been proposed to describe the pressure-saturation relation. They are generally empirical relations. One of the most commonly used functional forms is that of van Genuchten (1980):

$$\theta_w = \frac{\theta_{ws} - \theta_{wr}}{|1 + (\alpha h_c)^n|^{1 - \frac{1}{n}}} + \theta_{wr} \quad (\text{Eq. 1-8})$$

where θ_{ws} , θ_{wr} , α , n are used as fitting parameters with a given set of capillary pressure - saturation data. This functional form is favored by many numerical modelers as it is smooth, making it easier to handle numerically. Other functional forms such as that of Brooks and Corey (1964) have jump discontinuities in their derivatives which can cause numerical difficulties.

The functional form given above, which is the form used herein, ignores the effects of hysteresis. For more general imbibition-drainage problems it may be useful to include hysteresis. Several computational models have been developed by other authors including those of Kool and Parker (1987), and Moridis and Reddell (1991) who proposed a secondary water recovery system based on model results of unsaturated zone hysteresis. Hysteresis effects are ignored in this work.

Touma and Vauclin (1986) used van Genuchten's functional form to describe the pressure-saturation relationship in their column study of infiltration into coarse sand. Their experimentally fitted curve is determined by the relationship (Eq. 1-8) and the parameters:

$$\begin{aligned} \theta_{ws} &= 0.312 \text{ cm}^3/\text{cm}^3; & \theta_{wr} &= 0.0265 \text{ cm}^3/\text{cm}^3 \\ \alpha &= 0.044 \text{ cm}^{-1} & n &= 2.2 \end{aligned} \quad (\text{Eq. 1-9})$$

1-3. Constitutive relations

As the experiment was an infiltration experiment the saturated moisture content θ_{ws} is less than the porosity, which has a value of:

$$\phi = 0.37 \text{ cm}^3/\text{cm}^3$$

The difference is a measure of trapped air. This functional relationship is plotted in Figure 1-1.

The air fluid content can be found from the water content by noting that the sum of the fluid contents must be the volume of the void space:

$$\theta_w + \theta_a = \phi \quad (\text{Eq. 1-10})$$

or equivalently:

$$S_w + S_a = 1$$

The relative permeability is a function of fluid saturation. The function is usually determined empirically. To avoid the necessity of independently measuring a relative permeability-saturation relation, the functional form is often specified in terms of the parameters of the capillary pressure-saturation relation. For example, van Genuchten applied the theory of Mualem (1976) to his pressure-saturation relation (Eq. 1-8) to derive the equation:

$$k_{rw}(\theta_w) = \theta_e^{1/2} (1 - (1 - \theta_e^{1/m})^m)^2 \quad (\text{Eq. 1-11})$$

with:

$$m = 1 - 1/n$$

and the normalized water content (equivalent to the normalized saturation) defined by:

$$\theta_e = \frac{\theta_w - \theta_{wr}}{\theta_{ws} - \theta_{wr}}$$

van Genuchten did not derive the air phase relative permeability function in his work. This was done later by Parker (1987, 1989) who applied the theory of Mualem (1976) to the van Genuchten capillary pressure relation to find:

$$k_{ra}(\theta_w) = (1 - \theta_e)^{1/2} (1 - \theta_e^{1/m})^{2m} \quad (\text{Eq. 1-12})$$

Touma and Vauclin (1986) experimentally measured their relative permeability functions, preferring not to use a relationship inferred from the capillary pressure-saturation relation. Their water conductivity function was described with the fitted curve:

$$K_w = A_w \theta_w^{B_w} \quad (\text{Eq. 1-13})$$

with $A_w = 18130 \text{ cm/h}$ and $B_w = 6.07$. This leads to a saturated water conductivity of $K_{ws} = 15.40 \text{ cm/h}$ at the saturated moisture content of $\theta_{ws} = 0.312 \text{ cm}^3/\text{cm}^3$. The air conductivity is given by:

$$K_a = K_{as} \frac{A_a}{A_a + h_c^{B_a}} \quad (\text{Eq. 1-14})$$

with $A_a = 3.86 \times 10^{-5}$, $B_a = -2.4$ resulting in a value of air saturated conductivity of $K_{as} = 2800 \text{ cm/h}$. The pressure-saturation and relative permeability curves of Touma and Vauclin (1986) are illustrated in Figure 1-1.

The final constitutive equation specifies the relation between fluid density and fluid pressure. In this work the water phase is assumed to be essentially incompressible. The density of the air-phase is a function of air pressure. Two important factors affecting air density are neglected in this work: the effect of heat and the effect of contaminant concentration on air phase density. The air density is assumed to be a linear function of air pressure (Touma and Vauclin 1986):

$$\rho_a = \rho_{0a} \left(1 + \frac{h_a}{h_{0a}} \right) \quad (\text{Eq. 1-15})$$

with ρ_{0a} the density of the air phase at the pressure h_{0a} .

Figure 1-1 Capillary pressure and relative permeability as functions of saturation for the experimental data of Touma and Vauclin (1986).

1-4. Two-pressure equation formulation

(Eq. 1-1) and (Eq. 1-4) together with the constitutive relations specify the flow of the air and water phases. Given the system of equations there are many choices of independent variables. One of the most commonly measured hydrological variables is the fluid pressure head and so it is often the first choice of dependant variable for hydrologists. The two-pressure form of the flow equations are cast in terms of the two fluid pressures. The equations in this form are a direct statement of conservation of mass.

The previously derived mass balance equations will be rewritten as two equations, one for each of the water and air phases and expressed in terms of the phase pressure heads. The water equation will be considered first. The water mass balance equation (Eq. 1-1) is modified to account for elastic storage effects:

$$\phi \frac{\partial S_w}{\partial t} + S_{sw} S_w \frac{\partial h_w}{\partial t} + \nabla \cdot \mathbf{q}_w = F_w \quad (\text{Eq. 1-16})$$

In the above equation the water specific storativity S_{sw} has been introduced. The inclusion of the water storativity term in the equation ensures that the equation remains valid in the saturated zone where the derivative of water saturation is zero. In many models of the unsaturated zone the water compressibility is neglected and the storage term left out of the equation. This is

because the derivative of saturation $\frac{\partial S_w}{\partial t}$ is usually much larger than the term due to the compression of the water and solids

$S_{sw} S_w \frac{\partial h_w}{\partial t}$. In the above equation it has also been assumed that the water is only slightly compressible so that

$\mathbf{q}_w \cdot \nabla \rho_w \ll \rho_w \nabla \cdot \mathbf{q}_w$ and the term $\mathbf{q}_w \cdot \nabla \rho_w$ can be neglected.

Darcy's law is then substituted into (Eq. 1-16) to derive the final version of the water equation:

$$\frac{\partial \theta_w}{\partial t} + S_{sw} \frac{\partial h_w}{\partial t} - \nabla \cdot (K_w (\nabla h_w - \mathbf{i}_z)) = F_w \quad (\text{Eq. 1-17})$$

This equation is in mixed form. If the compressibility term is ignored then the temporal differentiation is applied to the moisture content and spatial differentiation is applied to the pressure head.

The air equation is written by expanding the time derivative of the mass balance equation (Eq. 1-3). The time derivative of air density is rewritten by substituting the equation relating air pressure to density (Eq. 1-15). The time derivative with respect to air content is changed to a derivative with respect to water content with the aid of (Eq. 1-10). Finally, Darcy's law (Eq. 1-6) is substituted for the fluid flux. The equation with these modifications is written:

$$(\phi - \theta_w) \frac{\rho_{0a}}{h_{0a}} \frac{\partial h_a}{\partial t} - \rho_a \frac{\partial \theta_w}{\partial t} - \nabla \cdot \left((\rho_a K_a) \left(\nabla h_a - \frac{\rho_a}{\rho_{ow}} \mathbf{i}_z \right) \right) = F_a \quad (\text{Eq. 1-18})$$

(Eq. 1-17) and (Eq. 1-18) will be referred to as the two-pressure formulation of the equations for the flow of air and water. The equations will be solved for the variables h_w and h_a . Darcy's law (Eq. 1-6) is used as a post process on the solutions h_w and h_a to find the fluid flux for each phase.

These equations are applied in both the unsaturated and saturated zones. In the saturated zone, the air is no longer present and the air equation (Eq. 1-18) is degenerate. The water equation decouples from the air equation and is solved for the water pressure head. The reverse will hold true in the case of a completely dry porous media.

Two types of boundary conditions can be specified for the equations for each fluid, either a first-type boundary condition of a fixed pressure head in the fluid, or second-type boundary condition of a specified fluid flux. Each equation requires one of these types of boundary conditions to be specified at every point on the spatial boundary of the domain. The paper by Touma and Vaucelin (1986) systematically reviews the effect of the boundary conditions in both an experimental column study and in a numerical model of the above equations in one dimension. Examples of the types of boundary conditions that can be specified for the two-pressure form of the equations will be discussed in the next section.

Source/sink terms appear on the right hand side of (Eq. 1-17) and (Eq. 1-18) and in this work they are assumed to be point sources and sinks. Such a description is convenient in developing numerical approximations of the equations as the source/sink terms can be located at discrete nodes of the mesh. The right hand side of the air and water equations are then written:

$$F_w^{n+1} = \sum_{j=1}^{No \text{ of wells}} Q_{w_j}^{n+1} \delta(x - x_j) \delta(z - z_j)$$

where the subscript j indexes the wells located at the nodes (x_j, z_j) and $\delta(z - z_j)$ is the delta function located at the node j .

The equations above are written with general operator notation. To expand the equation in cartesian geometry, the conductivity tensor must be described. It is assumed that the coordinate directions are aligned with the principle directions of the conductivity tensor. In two dimensions the conductivity tensor can be written:

$$K_w = \begin{bmatrix} K_{w_{xx}} & 0 \\ 0 & K_{w_{zz}} \end{bmatrix}$$

The water equation in two-dimensional (x, z) coordinates is written:

$$\frac{\partial \theta_w}{\partial t} + S_{sw} \frac{\theta_w}{\phi} \frac{\partial h_w}{\partial t} - \frac{\partial}{\partial x} \left[K_{w_{xx}} \frac{\partial h_w}{\partial x} \right] - \frac{\partial}{\partial z} \left[K_{w_{zz}} \left(\frac{\partial h_w}{\partial z} - \sin \psi \right) \right] = F_w \quad (\text{Eq. 1-19})$$

and the air equation:

$$\begin{aligned} & (\phi - \theta_w) \frac{\rho_{0a}}{h_{0a}} \frac{\partial h_a}{\partial t} - \rho_a \frac{\partial \theta_w}{\partial t} \\ & - \frac{\partial}{\partial x} \left[(\rho_a K_{a_{xx}}) \frac{\partial h_a}{\partial x} \right] - \frac{\partial}{\partial z} \left[(\rho_a K_{a_{zz}}) \left(\frac{\partial h_a}{\partial z} - \frac{\rho_a}{\rho_{ow}} \sin \psi \right) \right] \\ & = F_a \end{aligned} \quad (\text{Eq. 1-20})$$

1-5. Transport equations

With the flow of the two fluid phases specified, an equation for the transport of a contaminant must be written. The contaminant may be transported in either phase so an equation is written for each phase. The equations are mass balance statements. They employ the fluid velocity field obtained from the flow equations to specify the advective flux of the contaminant. The fluid velocity obtained from the flow equation is averaged in the sense that it does not account for differences of fluid velocity within each pore and between pores of the porous medium. These differences are accounted for by assuming a Fickian-type dispersive process. The equations also contain a term to account for reactive decay or production of the pollutant. The partitioning of the contaminant between the solid, liquid and gas phases will be discussed in a separate section. The validity of these equations is the subject of some debate (see for example Thorstenson and Pollock 1989). For a discussion of these equations and their derivation, the reader is referred to Bear (1979).

1-5-1. Governing equations

The amount of contaminant in each phase α is denoted by the mass fraction ω_α , which is defined as:

$$\omega_\alpha = \frac{\text{mass of contaminant in phase } \alpha}{\text{mass of phase } \alpha}$$

The mass balance equations for the transport of contaminants can then be written:

$$\begin{aligned} & \frac{\partial (\rho_\alpha \theta_\alpha \omega_\alpha)}{\partial t} + \nabla \cdot (\rho_\alpha q_\alpha \omega_\alpha) - \nabla \cdot (\theta_\alpha \rho_\alpha D_\alpha \cdot \nabla \omega_\alpha) + \lambda_\alpha \theta_\alpha \rho_\alpha \omega_\alpha \\ & = F^\alpha \end{aligned} \quad (\text{Eq. 1-21})$$

1-5. Transport equations

with the following notation:

- θ_α volumetric fluid content defined in (Eq. 1-2) $[L]^0$
- q_α volumetric flux of phase α $[L][T]^{-1}$
- λ_α reaction rate for phase α $[T]^{-1}$
- F^α source/sink term for phase α $[M][L]^{-3}[T]^{-1}$

In the transport equation (Eq. 1-21), the first term describes the change of contaminant mass in time, the second the movement of contaminant due to advection. The contaminants are assumed to be reactive with a decay rate of λ , and the right hand side describes sources and sinks in the equation. The dispersion in the third term is assumed to be Fickian in form with the dispersion tensor given by (Bear 1979):

$$D_{\alpha_{ij}} = \alpha_{T_\alpha} |v_\alpha| \delta_{ij} + (\alpha_{L_\alpha} - \alpha_{T_\alpha}) \frac{v_{\alpha_i} v_{\alpha_j}}{|v|} + D_{m_\alpha}^{eff} \delta_{ij}$$

with:

- $D_{\alpha_{ij}}$ i, j th components of the dispersivity tensor $[L]^2[T]^{-1}$
- α_T, α_L transverse and longitudinal dispersivities respectively $[L]$
- δ_{ij} the Kroneker delta ($\delta_{ij} = 1$ when $i=j$, 0 otherwise)
- v_α the flow velocity defined in (Eq. 1-7) $[L][T]^{-1}$
- $D_{m_\alpha}^{eff}$ the effective molecular diffusion coefficient $[L]^2[T]^{-1}$

For analysis of long-term transport problems, appropriate definition of the effective molecular diffusion coefficient for the air phase may be an important consideration. Effective molecular diffusion describes how free-air diffusion is reduced because of the reduction of surface area across which diffusion may take place. One-dimensional diffusive transport was described by Penman (1940) as a modified form of Fick's second law, with the effective diffusion coefficient given by

$$D_{m_a}^{eff} = D_{m_a} \theta_a \tau$$

where τ is the tortuosity, θ_a is the air content (volume of air/volume of voids), and D_{m_a} is the free-air diffusion coefficient.

Penman proposed a value of tortuosity of $\tau = 0.66$ for dry soils, based on laboratory experiments with several soils at various residual moisture contents. Experimental evidence indicates that the effective diffusion coefficient varies as a non-linear function of moisture content (Lai et al., 1976; Fluhler, 1973). The experimental results show that as moisture content increases to near saturation, the effective diffusion coefficient decreases dramatically. Lai et al. (1976) proposed the following formula:

$$D_{m_a}^{eff} = D_{m_a} \theta_a^{5/3}$$

Fluhler (1973) fit data empirically and arrived at the following relation, where τ_0 is the tortuosity at residual saturation.

$$D_{m_a}^{eff} = D_{m_a} \theta_a \tau_0 \left(\frac{\theta_a}{\phi} \right)^{3.25}$$

This relation yields an effective diffusion coefficient that is quite similar to the theoretical relation based on pore geometry proposed by Millington (1959). The formulation of Lai et al (1976), Fluhler (1973), and a typical free-air molecular diffusion coefficient are plotted in Figure 1-2. Examination the experimental data indicates that the data of Fluhler (1973) covers the largest range of saturation conditions. Because of this, the Fluhler equation is used in the simulations of section 3.

(Eq. 1-21) is written in conservative form. By expanding the derivatives in the first and second terms and making use of the flow equation (Eq. 1-1), the equation can be written in non-conservative form:

$$\rho_\alpha \theta_\alpha \frac{\partial \omega_\alpha}{\partial t} + \rho_\alpha q_\alpha \cdot \nabla \omega_\alpha - \nabla \cdot (\theta_\alpha \rho_\alpha D_\alpha \cdot \nabla \omega_\alpha) + \lambda_\alpha \theta_\alpha \rho_\alpha \omega_\alpha = F^\alpha$$

This form of the transport equation is useful as the hyperbolic part of the equation

$$\rho_\alpha \theta_\alpha \frac{\partial \omega_\alpha}{\partial t} + \rho_\alpha q_\alpha \cdot \nabla \omega_\alpha = 0$$

Figure 1-2 Effective molecular diffusion coefficient vs. Saturation of air, a comparison of formulations.

1-6. Contaminant partitioning

shows that the advective velocity of the pollutant is given by $v_\alpha = \frac{q_\alpha}{\theta_\alpha}$.

Rather than using the contaminant mass fraction it is often more convenient to use the volumetric concentration c_α which is defined as:

$$c_\alpha = \frac{\text{mass of contaminant in phase } \alpha}{\text{volume of phase } \alpha} = \rho_\alpha \omega_\alpha$$

In most of this work the contaminant concentration c_α will be used. The governing equations are rewritten in terms of c by substituting the above relation into the governing equations.

1-6. Contaminant partitioning

In this work it is assumed that there are three phases present in the unsaturated zone: the solid matrix, the liquid water phase and the gas phase. The contaminant can partition into each of these phases and there have been many studies and models developed of these processes. A review of these is beyond the scope of this work and only a few of the partitioning models will be considered here. These are sorption of the contaminant onto the solid phase, equilibrium vapor-liquid partitioning governed by Henry's law and kinetic mass transfer between the water and air phases. Literature reviews of other available models are provided by Weber et al. (1990), Gee et al. (1991), Miller et al (1991), and Mayer et al. (1992).

1-6-1. Sorption

Many pollutants are sorbed onto the solid phase and move at a rate slower than that predicted by the transport equations (see Eq. 1-21 and derived equations in section 1-5.) In the case of sorption the equation for the water phase is modified to include a retardation factor. The principle assumption used in deriving a retardation factor is that water is the wetting fluid so that the air phase does not have any contact with the solid phase. Thus adsorption can only occur from the water phase onto the solid phase. It is assumed that there is a Freundlich equilibrium isotherm between the water phase and the solid phase. The isotherm has the form:

$$\frac{\text{mass of contaminant in solid phase}}{\text{mass solid phase}} = F = k_d c_w$$

where k_d is called the distribution coefficient. The isotherm states that the concentration of contaminant in the solid phase is linearly proportional to that in the water phase. Typical values for this parameter can be found in the text by Domenico and Schwartz (1990). The amount of sorption is generally dependent on the contaminant and the composition of the soil. For example, organic contaminants are more strongly sorbed by soils having a higher degree of organic material. Using the assumption that sorption only occurs from the water to the solid phase, the equation for the water phase can be modified to include adsorption:

$$\frac{\partial(\theta_w c_w)}{\partial t} + \frac{\partial}{\partial t}(\theta_s \rho_s F) + \nabla \cdot (q_w c_w) - \nabla \cdot (\theta_w D_w \cdot \nabla c_w) + \lambda_w \theta_w c_w = F^w$$

where it is assumed that the water density is constant, and ρ_s and θ_s are the density and volumetric content of the solid phase. The time derivatives in the above equation can then be rewritten:

$$\frac{\partial(\theta_w c_w)}{\partial t} + \frac{\partial}{\partial t}(\theta_s \rho_s F) = \frac{\partial}{\partial t}(R \theta_w c_w)$$

where R is the retardation coefficient defined by:

$$R = \left(1 + \frac{\theta_s \rho_s k_d}{\theta_w} \right).$$

1-6-2. Vapor-liquid equilibria

The previous section described the sorption of a contaminant onto the solid phase from the liquid phase. Volatile contaminants also partition between the gas and liquid phases. Thus modeling the simultaneous transport of the contaminant in the water and air phases requires a description of the mass transfer processes between the phases. The most commonly made assumption is that the contaminant instantaneously establishes an equilibrium distribution between the phases. However, recent work (Cho and Jaffe 1990, 1993) has shown that significant dynamics may occur and that an equilibrium distribution takes some time to establish. In this case the phase exchange of mass follows a kinetic mass transfer law.

1-6-2-1. Equilibrium mass transfer

Under the equilibrium assumption, mass is assumed to exchange instantaneously between phases. The concentration in each phase is proportional to the concentration in the other phase. They are related by Henry's Law:

$$\frac{c_a}{c_w} = H$$

where H is called the Henry's constant. Henry's law is usually written in terms of the partial pressure of the contaminant in the vapor phase $P_c = K_H x_c$, where P_c is the partial pressure of the contaminant in the air phase, K_H is the Henry's law constant $[T^2]/[L][M]$, and x_c is the mole fraction of the contaminant in the water phase. By applying the ideal gas law and the definition of a mole fraction, H can be seen to be related to K_H by the following:

$$H = K_H \frac{MW_c MW_w}{\rho_w MW_c RT}$$

where MW is the molecular weight of either the contaminant or water, ρ_w is the density of water, R is the gas constant, and T the temperature in degrees Kelvin. Under the equilibrium assumption, the air concentration is directly proportional to the water concentration so the individual phase mass balance equations (Eq. 1-21) can be added to give one equation in water concentration:

$$\begin{aligned} & \frac{\partial ((R\theta_w + H\theta_a)\rho_w\omega_w)}{\partial t} + \nabla \cdot ((q_w + Hq_a)\rho_w\omega_w) - \\ & \nabla \cdot ((\theta_w\rho_w D_w + \theta_a H\rho_w D_a) \cdot \nabla \omega_w) - \nabla \cdot \theta_a \rho_a D_a \omega_w \nabla H' \\ & + (\lambda_w \theta_w + H\lambda_a \theta_a)\rho_w \omega_w \\ & = (F^w + F^a) \end{aligned}$$

The gradient of $H' = H \frac{\rho_w}{\rho_a}$ is assumed to be small and is neglected to give the equation:

$$\begin{aligned} & \frac{\partial ((R\theta_w + H\theta_a)c_w)}{\partial t} + \nabla \cdot ((q_w + Hq_a)c_w) - \\ & \nabla \cdot ((\theta_w D_w + \theta_a H D_a) \cdot \nabla c_w) + (\lambda_w \theta_w + H\lambda_a \theta_a)c_w \\ & = (F^w + F^a) \end{aligned} \tag{Eq. 1-22}$$

where it is assumed that the water density is constant.

1-6-2-2. Non-equilibrium partitioning

Cho and Jaffe (1990) conducted laboratory experiments that suggested an equilibrium assumption may not be valid in a dynamic system. Therefore, they developed a kinetic phase transfer model. Their experiments suggested that the contaminant moved from one phase to the other at a rate determined by the degree of disequilibrium, a kinetic phase transfer coefficient and the water content. For the transfer between phases they wrote the equations:

1-7. Discussion

$$\frac{dc_w}{dt} = K\theta_a(c_a - Hc_w)$$

$$\frac{dc_a}{dt} = -K\theta_a(c_a - Hc_w)$$

where K is the coefficient of mass transfer [L]/[T]. The mass transfer coefficient reflects the ease with which mass can move between the phases and will depend on the contaminant and porous medium properties. In the transport equation, the mass transfer equations appear as source and sink terms in the right hand side. When using kinetic mass transfer the transport equations for both phases must be used.

$$\begin{aligned} & \frac{\partial(\theta_w \rho_w \omega_w)}{\partial t} + \nabla \cdot (q_w \rho_w \omega_w) - \nabla \cdot (\theta_w \rho_w D_w \cdot \nabla \omega_w) + \lambda_w \theta_w \rho_w \omega_w \\ &= K\theta_a(\rho_a \omega_a - H\rho_w \omega_w) \\ & \frac{\partial(\theta_a \rho_a \omega_a)}{\partial t} + \nabla \cdot (q_a \rho_a \omega_a) - \nabla \cdot (\theta_a \rho_a D_a \cdot \nabla \omega_a) + \lambda_a \theta_a \rho_a \omega_a \\ &= -K\theta_a(\rho_a \omega_a - H\rho_w \omega_w) \end{aligned} \tag{Eq. 1-23}$$

This equation can be rewritten in terms of concentration. Assuming that the water density is constant and that:

$$\rho_a \nabla \omega_a \gg \omega_a \nabla \rho_a$$

then (Eq. 1-23) is written:

$$\begin{aligned} & \frac{\partial(\theta_w c_w)}{\partial t} + \nabla \cdot (q_w c_w) - \nabla \cdot (\theta_w D_w \cdot \nabla c_w) + \lambda_w \theta_w c_w = K\theta_a(c_a - Hc_w) \\ & \frac{\partial(\theta_a c_a)}{\partial t} + \nabla \cdot (q_a c_a) - \nabla \cdot (\theta_a D_a \cdot \nabla c_a) + \lambda_a \theta_a c_a = -K\theta_a(\rho_a \omega_a - H\rho_w \omega_w) \end{aligned} \tag{Eq. 1-24}$$

1-7. Discussion

For isothermal systems, the set of equations presented in this section provides a fairly general description of fluid flow and contaminant transport processes in the unsaturated zone. Fully dynamic water and air phases are represented, various descriptions of contaminant partitioning are included, and nonlinear air-phase diffusion coefficients are used. Because density changes due to temperature and concentration changes are not included, the flow equations are independent of the transport equations. This means that the coupled set of nonlinear flow equations can be solved before solving the transport equations, with Darcy's Law providing the velocity fields for each phase from the phase pressure solutions. This information then defines the parameters needed in the transport equation(s), which can then be solved.

For unsaturated flow and transport processes, different mathematical descriptions are appropriate for problems with different characteristic time scales. Within this document, two different time scales will be considered: short-time, defined as the time scale of an individual infiltration event; and long-time, defined as a time scale much longer than that of an individual infiltration event. For short-time problems, the full dynamics of the system will usually need to be included. In these cases, advection may be significant relative to diffusion, with individual phase velocities providing significant transport mechanisms. Partitioning kinetics are also likely to be important. For long-time problems, diffusion/dispersion processes will likely predominate, so the nonlinear expression for air-phase diffusion coefficient will be important. At long-time scales, partitioning kinetics should not be significant, with equilibrium being a reasonable description. In general, to study any specific field site, both short-time and long-time behavior must be understood. In this document, both types of behaviors will be described and modeled. All solutions are numerical, due to the complex nature of the governing equations. The next two sections describe

the numerical methods used for both flow and transport solutions. Within each section, examples are presented to demonstrate the numerical behaviors and to expose general behaviors of both short-term and long-term behaviors.

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2. Numerical solution of two-pressure equations

2-1. Introduction

While there have been many studies of water movement in the unsaturated zone, few have focussed on the movement of the air phase. Of those that have, most have ignored the influence of the water movement on the air phase. In this section a coupled air and water flow simulator is developed. The numerical technique used is that of Celia and Binning (1992). The contents of that paper are reproduced in this section in an expanded form. The work of Celia and Binning (1992) is an extension of the work of Celia et al. (1990a,b) on the Richards equation. The numerical model is used to study air flow in the unsaturated zone. The model is developed first in one dimension and later in two dimensions. The influence of heterogeneity on the air phase will be discussed, and mass flux vectors will be calculated for use in the contaminant transport model. Example problems will be drawn from the work of Touma and Vauclin (1986); other examples based on the experimental work in the unsaturated zone at Cape Cod, Massachusetts (Rudolph et al., 1993) may be found in Binning (1994).

The available literature on modeling multiphase flow in porous media spans a wide range of disciplines ranging from soil science through to petroleum engineering. The largest body of work on multiphase flow in porous media is in the petroleum literature. A review of some of this work is provided by Moridis and Reddell (1991) and Sleep and Sykes (1993). Petroleum problems differ from those in the unsaturated zone because of the high pressures that are present in deep porous formations. Boundary conditions for petroleum problems also tend to be quite different from those in the unsaturated zone.

For the reader interested in a wider review of the literature than the one here, there are many recent and comprehensive reviews on the subject of flow and transport in the unsaturated zone. These include: Gee et al. (1991) - flow and transport in the vadose zone; Abriola (1989) - the state of the art in multiphase migration of organic chemicals in groundwater; Vauclin (1989) - air and water flow models in the unsaturated zone. Milly (1988) - modelling of water in the unsaturated zone using Richards equation; Nielsen et al. (1986) - both flow and transport processes in the water phase in the unsaturated zone.

One of the major goals of this work is to investigate the importance of air phase movement in the unsaturated zone. The most common approach to multiphase flow and transport in the unsaturated zone is to assume an immobile air phase. Models using this assumption include those of Pinder and Abriola (1986), and Culver et al. (1991). While these models provide excellent results under many conditions, there has long been a questioning of the assumption of an immobile gas phase. For example, Green et al. (1970) were among the first to recognize the importance of the air phase in the unsaturated zone and include it in a one-dimensional two-phase finite difference model. However, the focus of many of the multiphase flow models of water and air movement in the unsaturated zone has been on the water phase. The objective of most previous research on two-phase air-water systems was to improve estimates of infiltration rates by including a dynamic air phase. A recent example of such a study is the work of Touma and Vauclin (1986) who observed the influence of the air phase on water movement both experimentally and with a one-dimensional finite difference model.

Recently there has been a renewed focus on air movement in the unsaturated zone. In large part this focus is motivated by the need to understand new technologies such as soil venting which pumps the air phase from the unsaturated zone in the hope of removing a volatile organic compound. To date there have only been a limited number of models of coupled air and water flow in the unsaturated zone. However, there are a large number of models that consider only the air phase, for example Johnson et al. (1990a) who assume a constant moisture content to derive analytical solutions of air movement. Others with this approach include Mohsen et al. (1980), Weeks et al. (1982), Baehr and Corapcioglu (1987), Metcalfe and Farquhar (1987), Mendoza and McAlary (1990), Mendoza and Frind (1990), Rathfelder et al. (1991), Benson et al. (1993), and McCarthy and Johnson (1993).

There are two principle difficulties associated with solving the governing equations. The first is that the equations are coupled through the fluid content which is a function of the capillary pressure, or the difference in pressure between the two fluids. The second difficulty in solving the equations is that they are non-linear. This can be seen as the fluid flux is the gradient of pressure head multiplied by the conductivity, which is a function of fluid content and thus also of pressure head. Any attempt to solve these equations must address each of these two fundamental features of the equations.

There are four predominant methodologies for the solution of the equations of multiphase flow. These can be grouped as (1) analytical methods, (2) finite difference methods, (3) finite element methods and (4) Lagrangian methods. Lagrangian methods recast the governing equations into an advection-diffusion form and solve the equations in a Lagrangian framework. This approach is not discussed further herein; for a detailed discussion, see Binning (1994).

Analytical solutions can only be obtained for these equations under strict assumptions. This makes their applicability quite limited. The solution is usually achieved by linearization of the equations and/or by decoupling the air and water equa-

tions. However, if the assumptions and limitations of these solutions are properly understood, analytical models can be powerful diagnostic tools that can give great insight into the situations where they are used. This is exemplified by the model of Johnson (1991), which combines a simple user interface with an analytical model of air flow to create a powerful tool for the initial evaluation of a venting scheme. There are many other analytical models of air and water flow in the unsaturated zone. They include the numerous solutions of Phillip (1965) (see Milly (1988) for a more extensive review of the work of Phillip), those of Brustkern and Morel-Seytoux (1970), Parlange and Hill (1979), Baehr (1987), Sander et al. (1988), and McWhorter and Sunada (1990).

The finite difference method is the most common technique for solving the equations. The strong tradition of the use of this method dates back to early applications to petroleum reservoir problems. Among the numerous users of this method are: Pinder and Abriola (1986) who solved the fully coupled three phase problem using an implicit finite difference model with a Newton Raphson non-linear iteration scheme, with the assumption of a constant-pressure immobile gas phase; Pruess (1987) with the coupled heat and mass flow model TOUGH; Sleep and Sykes (1989); Culver et al. (1991); Moridis and Reddell (1991); and Sleep and Sykes (1993) whose model is one of the most complete currently available. The model of Sleep and Sykes (1993) solves the fully coupled air and water flow equations and includes contaminant transport in both phases. The primary difference between their model and the one developed here is the numerical techniques used. The model of Sleep and Sykes and the model discussed in this work have essentially similar features.

The finite element method is favored by many authors for its flexibility in dealing with boundary conditions and for its ability to handle non-rectangular domains and elements. Often the finite element method can be made to appear identical to a finite difference method by judicious choice of test and trial functions. The finite element method has been applied to the multiphase flow problem by far fewer authors than have chosen the finite difference method. This may be historical, as there is a strong bias towards finite difference methods among petroleum engineers who did much of the pioneering work in unsaturated zone hydrology. Finite difference methods are also particularly simple and intuitive. In this work the finite element method is chosen because of its flexibility. Among the authors employing the finite element method are: Kaluarachchi and Parker (1989); Mendoza and Frind (1990); and Schrefler and Xiaoyong (1993) who also included consolidation of the solid phase in their work.

The principle difficulties in solving the equations lie in the linearization procedure and the method for dealing with the coupling between the equations. The most comprehensive study of the non-linearity in the unsaturated flow equations is the study of Paniconi et al. (1991). They analyzed a variety of approaches to the linearization of Richards equation. In their work, it was apparent that the methods performed differently for each example problem considered, making any comparison between them difficult. Kaluarachchi and Parker (1989) also compared the Picard and Newton Raphson iteration schemes for modelling multiphase flow. They found that the performance of the two methods depended on the overall numerical approximation. For instance they found that Picard iteration performed better than a Newton Raphson scheme if upstream weighting was used and found the opposite if it was not. In this work the Picard iteration scheme will be used. The Picard iteration scheme may not be the most efficient linearization scheme for some problems. However, it is extremely robust, providing solutions in situations where other methods would fail to converge. It is also very simple, which makes it easy to implement and explain to the user of the model.

The other difficulty that must be overcome is the coupling between the air and water equations. A common approach is to decouple the equations. This is the heart of the implicit pressure, explicit saturation (IMPES) strategy used in the petroleum industry. The IMPES scheme solves the equations implicitly in pressure of one phase, explicitly in saturation of the other, thus decoupling the equations. The IMPES was used by Phuc and Morel-Seytoux (1972). The work of Sleep and Sykes (1989) also used the IMPES, solving the Richards equation for the water phase and then explicitly calculating the behavior of the air phase. In a more recent work, Sleep and Sykes (1993) compared the accuracy and efficiency of both an IMPES scheme and a fully implicit scheme. They found that the IMPES was more restricted in time step size than the fully implicit scheme. The difference in time step size made up for any advantage in speed the IMPES solution gained by decoupling the equations. However, the IMPES scheme requires less memory, which may be a consideration for larger problems. The IMPES works best where there is little coupling between the air and water phases. This is true for the majority of commonly occurring boundary conditions. However, the column study of Touma and Vauclin (1986) shows that if the air is trapped by the infiltrating water, it will significantly retard the water movement. An IMPES type solver should be expected to be a poor predictor of this type of behavior. The accuracy of the IMPES is also dependant upon the strength of the non-linearities in the equation. In the vicinity of steep pressure gradients such as those that occur at an infiltrating front, the non-linearities are strong. In this work the equations will be solved using a fully implicit coupled scheme.

The multiphase flow equations written with the two fluid pressures as the dependant variables are similar in form to the Richards equation. The numerical method used in this section extend previous work on Richards equation, adapting the methods for multiphase flow. Many approaches have been used to solve Richards equation, dating back to the work by Freeze (1971). Richards equation is known to be difficult to solve with the most difficult problems being those of infiltration into an initially dry soil, involving very steep pressure gradients. Recently, Celia et al. (1990) identified two issues as being important

in the numerical solution of Richards equation. The first is the equation form which is important for the mass balance of the resulting numerical approximation, and the second is the numerical treatment of the temporal derivative.

The mass balance of a numerical approximation of Richards equation is dependant on the form of the governing equation. The form of the governing equation is decided by the choice of dependant variable with the two common choices being the pressure head and moisture content. The formulation based on the moisture content possesses excellent mass balance properties. It works well in the unsaturated zone, but is not applicable in the saturated zone as the moisture content is constant there. The pressure-head-based form of the equation is valid in the saturated zone, but does not conserve mass. Celia et al. (1990) demonstrated these behaviors numerically and showed that numerical approximations based on the mixed equation form possesses the advantages of both methods. In the mixed form of the equation the time derivative is written in terms of the moisture content and the spatial derivatives in terms of the pressure head. A numerical scheme based on these equations is mass conservative and also valid in the saturated zone. The mixed form of the flow equation will be used in this work for each of the two phases.

The treatment of the time derivative in a numerical approximation of Richards equation is equally important to the success of the method. This was first noted by Neuman (1973), later by Milly (1985), Bouloutas (1989), Ross (1990) and Celia et al. (1990). They showed the benefits of lumping of the finite element discretization of the time derivative. If the finite element discretization is used without mass lumping the approximation does not obey a maximum principle and oscillations result. In practice this is most important around steep pressure fronts where the consistent approximation produces large oscillations. For sufficiently steep fronts, the oscillations are so large that the non-linear iteration scheme does not converge. A lumped scheme will often give good solutions in these instances. Celia et al. (1990) concluded that a combination of mass lumping with the mixed form of the equations is the most effective method for solution of the Richards equation.

Richards equation serves as an excellent model for the multiphase flow equations because each phase equation closely resembles Richards equation. In the next section the extension of the Richards equation work to the multiphase flow problem is discussed.

2-2. Numerical solution in one dimension

The solution of the two-phase flow equations in one dimension is given in Celia and Binning (1992). The governing equations for the flow problem were stated in section 1. The equations in one dimension are written ((Eq. 1-17) and (Eq. 1-18)):

$$\frac{\partial \theta_w}{\partial t} + S_{sw} \frac{\theta_w}{\phi} \frac{\partial h_w}{\partial t} - \frac{\partial}{\partial z} \left[K_w \left(\frac{\partial h_w}{\partial z} - \sin \psi \right) \right] = 0 \quad (\text{Eq. 2-1})$$

and

$$(\phi - \theta_w) \frac{\rho_{0a}}{h_{0a}} \frac{\partial h_a}{\partial t} - \rho_a \frac{\partial \theta_w}{\partial t} - \frac{\partial}{\partial z} \left[(\rho_a K_a) \left(\frac{\partial h_a}{\partial z} - \frac{\rho_a}{\rho_{ow}} \sin \psi \right) \right] = 0 \quad (\text{Eq. 2-2})$$

where ψ is the angle away from the vertical.

2-2-1. Temporal discretization: Modified Picard iteration scheme

The numerical scheme is based on the work of Celia et al. (1990). The air and water equations are discretized using a modified Picard approach. The equations are discretized in time with an Euler backward difference scheme. The scheme is fully implicit and thus is the most stable form of temporal discretization. Picard iteration is used to linearize the equations:

$$\frac{\Theta_w^{n+1,m+1} - \Theta_w^n}{\Delta t} + S_{sw} \frac{\Theta_w^{n+1,m} H_w^{n+1,m+1} - H_w^n}{\phi \Delta t} - \frac{\partial}{\partial z} \left[K_w^{n+1,m} \left(\frac{\partial H_w^{n+1,m+1}}{\partial z} - \sin \psi \right) \right] = 0 \quad (\text{Eq. 2-3})$$

$$(\phi - \Theta_w^{n+1,m}) \frac{\rho_{0a} H_a^{n+1,m+1} - H_a^n}{h_{0a} \Delta t} - \rho_a^{n+1,m} \frac{\Theta_w^{n+1,m+1} - \Theta_w^n}{\Delta t} - \frac{\partial}{\partial z} \left[(\rho_a K_a)^{n+1,m} \left(\frac{\partial H_a^{n+1,m+1}}{\partial z} - \frac{\rho_a^{n+1,m}}{\rho_{ow}} \sin \psi \right) \right] = 0 \quad (\text{Eq. 2-4})$$

In equations (Eq. 2-3) and (Eq. 2-4) the superscript n denotes the time level, m denotes the iteration level,

$\Delta t = t^{n+1} - t^n$ is the time step size, and Θ_w , H_w and H_a are the numerical approximations to the moisture content θ_w and the pressure heads h_w and h_a respectively. At each time step the solution is iterated until the pressure head converges. During each iteration the equations are solved to find the pressure heads at the new iteration level. The nonlinear coefficients are evaluated using the pressure heads at the old iteration level thus linearizing the equations. The moisture content Θ_w^{n+1} is written at the m th iteration level when it multiplies $H_w^{n+1,m+1}$ and at the $m+1$ th iteration level when it does not. Because the equations will be solved for the pressure head at the new iteration level, the moisture content at the new iteration level must be written in terms of the pressure head at the new iteration level. This is achieved by use of the following Taylor series expansion so that:

$$\Theta_w^{n+1,m+1} \approx \Theta_w^{n+1,m} + \left(\frac{d\theta_w}{dh_c} \right)^{n+1,m} (H_c^{n+1,m+1} - H_c^{n+1,m}) \quad (\text{Eq. 2-5})$$

In the above $\left(\frac{d\theta_w}{dh_c} \right)^{n+1,m}$ is found by evaluating the derivative of the moisture content function $C_w = \frac{d\theta_w}{dh_c}$ with the capillary pressure head at the old iteration level $H_c^{n+1,m}$. The derivative of the moisture content function is denoted by C_w and is called the specific moisture capacity function.

It is useful to recast (Eq. 2-3) and (Eq. 2-4) in terms of the increment in pressure at each iteration level:

$$\delta H_a^{n+1,m} = H_a^{n+1,m+1} - H_a^{n+1,m} \quad (\text{Eq. 2-6})$$

Using the Taylor expansion (Eq. 2-5) and the definition (Eq. 2-6) the equations are then written:

$$\begin{aligned}
 & C_w^{n+1,m} \frac{\delta H_a^{n+1,m} - \delta H_w^{n+1,m}}{\Delta t} + S_{sw} \frac{\Theta_w^{n+1,m}}{\phi} \frac{\delta H_w^{n+1,m}}{\Delta t} \\
 & - \frac{\partial}{\partial z} \left(K_w^{n+1,m} \frac{\partial \delta H_w^{n+1,m}}{\partial z} \right) \\
 & = - \frac{\Theta_w^{n+1,m} - \Theta_w^n}{\Delta t} - S_{sw} \frac{\Theta_w^{n+1,m}}{\phi} \frac{H_w^{n+1,m} - H_w^n}{\Delta t} \\
 & + \frac{\partial}{\partial z} \left[K_w^{n+1,m} \left(\frac{\partial H_w^{n+1,m}}{\partial z} - \sin \psi \right) \right] \\
 & \equiv R_w^{n+1,m}
 \end{aligned} \tag{Eq. 2-7}$$

and

$$\begin{aligned}
 & (\phi - \Theta_w^{n+1,m}) \frac{\rho_{0a}}{h_{0a}} \frac{\delta H_a^{n+1,m}}{\Delta t} - \rho_a^{n+1,m} C_w^{n+1,m} \frac{\delta H_a^{n+1,m} - \delta H_w^{n+1,m}}{\Delta t} \\
 & - \frac{\partial}{\partial z} \left[(\rho_a K_a)^{n+1,m} \frac{\partial \delta H_a^{n+1,m}}{\partial z} \right] \\
 & = \rho_a^{n+1,m} \frac{\Theta_w^{n+1,m} - \Theta_w^n}{\Delta t} - (\phi - \Theta_w^{n+1,m}) \frac{\rho_{0a}}{h_{0a}} \frac{H_a^{n+1,m} - H_a^n}{\Delta t} \\
 & + \frac{\partial}{\partial z} \left[(\rho_a K_a)^{n+1,m} \frac{\partial H_a^{n+1,m}}{\partial z} - \frac{(\rho_a^{n+1,m})^2}{\rho_{0w}} K_a^{n+1,m} \sin \psi \right] \\
 & \equiv R_a^{n+1,m}
 \end{aligned} \tag{Eq. 2-8}$$

At each iteration the equations are solved for the increment in pressure during the iteration $\delta H_a^{n+1,m}$. The equations are linear in $\delta H_a^{n+1,m}$, and $\delta H_a^{n+1,m}$ appears only on the left hand side of each equation. After the solution is obtained, the pressure at the new iteration level is updated using (Eq. 2-6).

Convergence of the iteration scheme is checked by two measures. The first measure of convergence is that the increment in pressure head $\delta H_a^{n+1,m}$ at each iteration step goes to zero as the solution converges. The second check is that the right hand side of the equation $R_a^{n+1,m}$ goes to zero. As the iteration scheme converges the right hand side of each equation gives a direct measure of how well the solution $H_a^{n+1,m}$ satisfies the discrete version of the governing equation.

To complete the discretization a spatial approximation is required. A lumped Galerkin finite element scheme with piecewise linear basis functions is chosen. This spatial discretization with lumping of the time derivative is equivalent to a centered-in-space finite difference scheme in one dimension, given appropriate choices for interblock conductivity estimates.

2-2-2. Spatial discretization: Galerkin finite element scheme

The water equation is considered first. The weak form of equation (Eq. 2-7) is:

2-2. Numerical solution in one dimension

$$\begin{aligned}
 & \int_{\Omega_z} \left\{ C_w^{n+1,m} \frac{\delta H_a^{n+1,m} - \delta H_w^{n+1,m}}{\Delta t} + S_{sw} \frac{\Theta_w^{n+1,m}}{\phi} \frac{\delta H_w^{n+1,m}}{\Delta t} \right. \\
 & \quad \left. - \frac{\partial}{\partial z} \left(K_w^{n+1,m} \frac{\partial \delta H_w^{n+1,m}}{\partial z} \right) \right\} w \, dz \\
 &= \int_{\Omega_z} \left\{ \left(- \frac{\Theta_w^{n+1,m} - \Theta_w^n}{\Delta t} - S_{sw} \frac{\Theta_w^{n+1,m}}{\phi} \frac{H_w^{n+1,m} - H_w^n}{\Delta t} \right) \right. \\
 & \quad \left. + \frac{\partial}{\partial z} \left[K_w^{n+1,m} \left(\frac{\partial H_w^{n+1,m}}{\partial z} - \sin \psi \right) \right] \right\} w \, dz
 \end{aligned}$$

where w is the test function, and $\Omega_z = [0, l]$ is the spatial domain ranging from $z=0$ to $z=l$. The divergence of flux in the weak form of the equation is integrated by parts. This is convenient as it introduces the boundary conditions into the equation in a natural way:

$$\begin{aligned}
 & \int_{\Omega_z} \left\{ C_w^{n+1,m} \frac{\delta H_a^{n+1,m} - \delta H_w^{n+1,m}}{\Delta t} + S_{sw} \frac{\Theta_w^{n+1,m}}{\phi} \frac{\delta H_w^{n+1,m}}{\Delta t} \right\} w \, dz \\
 & + \int_{\Omega_z} \left\{ K_w^{n+1,m} \frac{\partial \delta H_w^{n+1,m}}{\partial z} \frac{\partial w}{\partial z} \right\} dz \\
 &= \int_{\Omega_z} \left\{ - \frac{\Theta_w^{n+1,m} - \Theta_w^n}{\Delta t} - S_{sw} \frac{\Theta_w^{n+1,m}}{\phi} \frac{H_w^{n+1,m} - H_w^n}{\Delta t} \right\} w \, dz \\
 & + [q_w^{n+1} w]_0^l - \int_{\Omega_z} K_w^{n+1,m} \left(\frac{\partial H_w^{n+1,m}}{\partial z} - \sin \psi \right) \frac{\partial w}{\partial z} dz
 \end{aligned}$$

In the above, the term:

$$\left[K_w^{n+1,m} \frac{\partial \delta H_w^{n+1,m}}{\partial z} w \right]_0^l$$

has been neglected (on the left side of the equation) because $\delta h_w \rightarrow 0$ as the iteration scheme converges.

The finite-dimensional trial and test space are defined by partitioning the domain into $N-1$ elements (z_1^e, z_2^e) , where z_1^e and z_2^e are the coordinates of the left and right boundaries of the element e . The trial and test functions are chosen to be the space of piecewise linear functions which are defined in local coordinates by the basis functions:

$$\phi_1(\zeta) = \frac{1-\zeta}{2} \quad \phi_2(\zeta) = \frac{1+\zeta}{2}$$

where the local coordinate is related to the global coordinate system by:

$$\zeta = \frac{2z - (z_1^e + z_2^e)}{z_2^e - z_1^e}$$

These functions are illustrated in Figure 2-1.

The trial space is used to approximate the solution h_α and the coefficients as follows:

Figure 2-1 Basis functions for the one-dimensional finite element solution of the flow equation.

$$h_w(z, t) \approx \sum_{j=1}^N H_{w_j}(t) \phi_j(z)$$

$$K_w(h_c) \approx \sum_{j=1}^N K_w(H_{c_j}) \phi_j(z) = \sum_{j=1}^N K_{w_j} \phi_j(z)$$

$$C_w(h_c) \approx \sum_{j=1}^N C_{w_j} \phi_j$$

$$\theta_w \approx \sum_{j=1}^N \Theta_{w_j} \phi_j$$

The integrals are evaluated elementwise, so that:

$$\int_0^l dz = \sum_{e=1}^{N-1} \int_{z_i^e}^{z_2^e} dz$$

With these definitions the element integrals are written:

$$\begin{aligned} & \sum_{k=1}^N \sum_{j=1}^N \sum_{i=1}^N C_{w_k}^{n+1,m} \frac{\delta H_{a_j}^{n+1,m} - \delta H_{w_j}^{n+1,m}}{\Delta t} A_{ijk}^e \\ & + \sum_{k=1}^N \sum_{j=1}^N \sum_{i=1}^N S_{sw} \frac{\Theta_{w_k}^{n+1,m} \delta H_{w_j}^{n+1,m}}{\phi} \frac{1}{\Delta t} A_{ijk}^e \\ & + \sum_{k=1}^N \sum_{j=1}^N \sum_{i=1}^N K_{w_k}^{n+1,m} \delta H_{w_j}^{n+1,m} B_{ijk}^e \end{aligned}$$

$$\begin{aligned}
&= - \sum_{j=1}^N \sum_{i=1}^N \frac{\Theta_{w_j}^{n+1,m} - \Theta_{w_j}^n}{\Delta t} D_{ij}^e \\
&\quad - \sum_{k=1}^N \sum_{j=1}^N \sum_{i=1}^N S_{sw} \frac{\Theta_{w_k}^{n+1,m} H_{w_j}^{n+1,m} - H_{w_j}^n}{\phi \Delta t} A_{ijk}^e \\
&\quad + [q_w^{n+1} v]_{z_1^e}^{z_2^e} - \left(\sum_{k=1}^N \sum_{j=1}^N \sum_{i=1}^N K_{w_k}^{n+1,m} H_{w_j} B_{ijk}^e - \sum_{k=1}^N \sum_{i=1}^N K_{w_k}^{n+1,m} E_{ik}^e \sin \psi \right)
\end{aligned}$$

where:

$$A_{ijk}^e = \int_{z_1^e}^{z_2^e} \phi_k \phi_j \phi_i dz = \begin{cases} \frac{(z_2^e - z_1^e)}{12} \begin{bmatrix} 3 & 1 \\ 1 & 1 \end{bmatrix} & k = 1 \\ \frac{(z_2^e - z_1^e)}{12} \begin{bmatrix} 1 & 1 \\ 1 & 3 \end{bmatrix} & k = 2 \end{cases}$$

$$B_{ijk}^e = \int_{z_1^e}^{z_2^e} \phi_k \frac{\partial \phi_j}{\partial z} \frac{\partial \phi_i}{\partial z} dz = \frac{1}{2(z_2^e - z_1^e)} \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}$$

$$D_{ij}^e = \int_{z_1^e}^{z_2^e} \phi_j \phi_i dz = \frac{(z_2^e - z_1^e)}{6} \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix}$$

$$E_{ik}^e = \int_{z_1^e}^{z_2^e} \phi_k \frac{\partial \phi_i}{\partial z} dz = \frac{1}{2} \begin{bmatrix} -1 & -1 \\ 1 & 1 \end{bmatrix}$$

With these matrix definitions the final global approximation can be assembled. The first term of the equation at node i is written:

$$\begin{aligned}
&\frac{\bar{C}_{w_{i-1}}^{n+1,m}}{\Delta t} (\delta H_{a_{i-1}}^{n+1,m} - \delta H_{w_{i-1}}^{n+1,m}) \\
&+ \frac{\bar{C}_{w_i}^{n+1,m}}{\Delta t} (\delta H_{a_i}^{n+1,m} - \delta H_{w_i}^{n+1,m}) \\
&+ \frac{\bar{C}_{w_{i+1}}^{n+1,m}}{\Delta t} (\delta H_{a_{i+1}}^{n+1,m} - \delta H_{w_{i+1}}^{n+1,m})
\end{aligned} \tag{Eq. 2-9}$$

where:

$$\bar{C}_{w_{i-1}}^{n+1,m} = \frac{1}{12} (C_{w_{i-1}}^{n+1,m} + C_{w_i}^{n+1,m})$$

$$\bar{C}_{w_i}^{n+1,m} = \frac{1}{12} (C_{w_{i-1}}^{n+1,m} + 6C_{w_i}^{n+1,m} + C_{w_{i+1}}^{n+1,m})$$

$$\bar{C}_{w_{i+1}}^{n+1,m} = \frac{1}{12} (C_{w_i}^{n+1,m} + C_{w_{i+1}}^{n+1,m})$$

As can be seen in the above equation, the approximation of the temporal derivative is distributed in space around nodes $i-1$, i , $i+1$. Celia et al. (1990) and others identified this distribution of mass as the source of the oscillations that are present in the solution.

2-2-3. Temporal lumping

The oscillations in the solution can be eliminated, or greatly reduced in size by employing a temporal lumping scheme. Bouloutas (1989) analyzed a finite element discretization of the heat equation:

$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2}$$

He demonstrated that the lumped finite element scheme of this equation obeys a maximum principle. The solution can be shown to attain a maximum at the initial time $t=0$ or at the boundaries so that oscillations do not occur. Bouloutas noted the similarity between the heat equation and Richards' equation. The analysis of the heat equation is a useful guide. However, the multiphase flow equations are highly non-linear, and although the oscillations are greatly reduced they are not necessarily eliminated altogether.

The lumping scheme used here is the L_2 scheme of Milly (1985). Milly replaces the term:

$$\sum_{j=1}^N \frac{\delta H_{w_j}^{n+1, m+1}}{\Delta t} \int_{\Omega_z} \hat{C}_w \phi_j \phi_i dz$$

(where $\hat{C}_w$ is the numerical approximation to C_w) with:

$$\frac{\delta H_{w_i}^{n+1, m+1}}{\Delta t} C_{w_i}^{n+1, m} \int_{\Omega_z} \phi_i dz$$

The effect of the lumping scheme is to diagonalize the temporal matrix. The approximation of (Eq. 2-9) is replaced with:

$$C_{w_i}^{n+1, m} \frac{\delta H_{a_i}^{n+1, m+1} - \delta H_{w_i}^{n+1, m+1}}{\Delta t}$$

The other temporal terms can be treated in the same way.

For constant grid spacing Δz , the final discrete version of the equation at interior node i is written:

$$\begin{aligned} & \frac{C_{w_i}^{n+1, m}}{\Delta t} (\delta H_{a_i}^{n+1, m+1} - \delta H_{w_i}^{n+1, m+1}) + S_{sw} \frac{\Theta_{w_i}^{n+1, m} \delta H_{w_i}^{n+1, m}}{\phi \Delta t} \\ & - \frac{1}{\Delta z^2} [K_{w_{i+1/2}}^{n+1, m} (\delta H_{w_{i+1}}^{n+1, m} - \delta H_{w_i}^{n+1, m}) - K_{w_{i-1/2}}^{n+1, m} (\delta H_{w_i}^{n+1, m} - \delta H_{w_{i-1}}^{n+1, m})] \\ & = - \frac{\Theta_{w_i}^{n+1, m} - \Theta_{w_i}^n}{\Delta t} - S_{sw} \frac{\Theta_{w_i}^{n+1, m} H_{w_i}^{n+1, m} - H_{w_i}^n}{\phi \Delta t} \\ & + \frac{1}{\Delta z^2} [K_{w_{i+1/2}}^{n+1, m} (H_{w_{i+1}}^{n+1, m} - H_{w_i}^{n+1, m}) - K_{w_{i-1/2}}^{n+1, m} (H_{w_i}^{n+1, m} - H_{w_{i-1}}^{n+1, m})] \\ & - \frac{K_{w_{i+1/2}}^{n+1, m} - K_{w_{i-1/2}}^{n+1, m}}{\Delta z} \sin \psi \end{aligned} \quad (\text{Eq. 2-10})$$

where:

$$K_{\alpha_{i\pm 1/2}}^{n+1, m} = \frac{1}{2} (K_{\alpha_{i\pm 1}}^{n+1, m} + K_{\alpha_i}^{n+1, m})$$

2-2. Numerical solution in one dimension

The air equation is developed in a similar manner:

$$\begin{aligned}
 & (\phi - \Theta_{w_i}^{n+1,m}) \frac{\rho_{0a} \delta H_{a_i}^{n+1,m}}{h_o \Delta t} - \rho_{a_i}^{n+1,m} \frac{C_{w_i}^{n+1,m}}{\Delta t} (\delta H_{a_i}^{n+1,m+1} - \delta H_{w_i}^{n+1,m+1}) \\
 & - \frac{1}{\Delta z^2} [(\rho_a K_a)_{i+1/2}^{n+1,m} (\delta H_{a_{i+1}}^{n+1,m} - \delta H_{a_i}^{n+1,m})] \\
 & + \frac{1}{\Delta z^2} [(\rho_a K_a)_{i-1/2}^{n+1,m} (\delta H_{a_i}^{n+1,m} - \delta H_{a_{i-1}}^{n+1,m})] \\
 & = \rho_{a_i}^{n+1,m} \frac{\Theta_{w_i}^{n+1,m} - \Theta_{w_i}^n}{\Delta t} - (\phi - \Theta_{w_i}^{n+1,m}) \frac{\rho_{0a} H_{a_i}^{n+1,m} - H_{a_i}^n}{h_{0a} \Delta t} \\
 & + \frac{1}{\Delta z^2} [(\rho_a K_a)_{i+1/2}^{n+1,m} (H_{a_{i+1}}^{n+1,m} - H_{a_i}^{n+1,m}) - (\rho_a K_a)_{i-1/2}^{n+1,m} (H_{a_i}^{n+1,m} - H_{a_{i-1}}^{n+1,m})] \\
 & - \frac{\left(\frac{\rho_a^2}{\rho_{0w}} K_a \right)_{i+1/2}^{n+1,m} - \left(\frac{\rho_a^2}{\rho_{0w}} K_a \right)_{i-1/2}^{n+1,m}}{\Delta z} \sin \psi
 \end{aligned} \tag{Eq. 2-11}$$

In one dimension the lumped Galerkin finite element discretization with piecewise linear basis functions is equivalent to a centered-in-space finite difference scheme. In the equivalent finite difference scheme the conductivity function at the midpoint of elements is evaluated with an arithmetic average.

When the equations are assembled into matrix form, the resulting matrix of algebraic equations is banded in structure.

The water equation at node i contains $\delta H_w^{n+1,m+1}$ at nodes $i-1, i, i+1$ and $\delta H_a^{n+1,m+1}$ at node i . The air equation has a similar form. The air and water equations are interleaved, with the water equation at node i being followed by the air equation at node i and the resultant matrix is pentadiagonal in structure that is suitable for banded matrix storage and solution.

2-2-4. Boundary conditions

Two types of boundary conditions can be specified. First-type boundary conditions of a fixed pressure head in either phase can be specified by replacing the discrete finite element equation at the boundary node by the statement that:

$$\delta H_\alpha^{n+1,m+1} = 0$$

The value of $H_\alpha^{n+1,m}$ on the boundary at the new time level must also be set to be the value of the pressure boundary condition to ensure that the correct solution is obtained. $H_\alpha^{n+1,m}$ needs only to be specified at the beginning of each time step for a fixed head condition. After each iteration step the solution is updated by using the relation (Eq. 2-6):

$$H_\alpha^{n+1,m+1} = H_\alpha^{n+1,m} + \delta H_\alpha^{n+1,m}$$

Since the boundary condition is specified with $\delta H_\alpha^{n+1,m+1} = 0$ the value of the pressure which is fixed at the boundary remains the same at each iteration step.

Flux boundary conditions are specified by including the additional boundary term $[q_w^{n+1} \phi_i]_0^l$ which is present in the finite element equation at the boundary. An equivalent finite difference boundary condition can be found as follows. For example, consider a flux boundary condition in the water phase at the top of the domain. If the first node in the domain is numbered 1 a hypothetical node is introduced outside the domain, which will be denoted as node 0. The flux in the water phase at

the boundary node is the average of the flux on either side of the boundary at distance $\frac{\Delta z}{2}$:

$$q_w^{top} = \frac{q_{w_{1/2}} + q_{w_{1+1/2}}}{2}$$

The flux is approximated using a centred-in-space difference scheme so that:

$$q_w^{top} = -\frac{1}{2} \left(K_{w_{1+1/2}}^{n+1,m} \frac{H_{w_2}^{n+1,m} - H_{w_1}^{n+1,m}}{\Delta z} - K_{w_{1+1/2}}^{n+1,m} \sin \psi \right) - \frac{1}{2} \left(K_{w_{1/2}}^{n+1,m} \frac{H_{w_1}^{n+1,m} - H_{w_0}^{n+1,m}}{\Delta z} - K_{w_{1/2}}^{n+1,m} \sin \psi \right)$$

This equation is solved for the pressure at the hypothetical node 0. The result is used to eliminate $H_{w_0}^{n+1,m}$ from the finite difference equation (Eq. 2-10) written at node 1. The resultant water equation at the top boundary is:

$$\begin{aligned} & \frac{C_{w_i}^{n+1,m}}{\Delta t} (\delta H_{a_1}^{n+1,m+1} - \delta H_{w_1}^{n+1,m+1}) + S_{sw} \frac{\Theta_{w_1}^{n+1,m} \delta H_{w_1}^{n+1,m}}{\phi \Delta t} \\ & - \frac{2}{\Delta z^2} [K_{w_{1+1/2}}^{n+1,m} (\delta H_{w_2}^{n+1,m} - \delta H_{w_1}^{n+1,m})] \\ & = - \frac{\Theta_{w_1}^{n+1,m} - \Theta_{w_1}^n}{\Delta t} - S_{sw} \frac{\Theta_{w_1}^{n+1,m} H_{w_1}^{n+1,m} - H_{w_1}^n}{\phi \Delta t} \\ & + \frac{2}{\Delta z^2} [K_{w_{1+1/2}}^{n+1,m} (H_{w_2}^{n+1,m} - H_{w_1}^{n+1,m})] \\ & + \frac{2(q_w^{top})^{n+1}}{\Delta z} - \frac{2K_{w_{1+1/2}}^{n+1,m}}{\Delta z} \sin \psi \end{aligned} \quad (\text{Eq. 2-12})$$

The finite element boundary condition and the finite difference boundary conditions derived through this method are equivalent.

2-2-5. Mass balance

In the previous section the finite element equation at the top boundary was given (Eq. 2-10). When the Picard iteration scheme converges the left hand side of the equation goes to zero. The right hand side is a discrete version of the governing equation at the top boundary and it can be solved for the flux of water at the top boundary $(q_w^{top})^{n+1}$. A similar procedure can be used to find the flux at the bottom in the water phase and the boundary flux in the air phase. The boundary flux is used to evaluate the mass balance. The mass balance ratio at each time step is defined as the change of mass in the domain divided by the flux into the domain at the boundaries:

$$\text{mass balance ratio in water} = \frac{\sum_{i=1}^N (\Theta_i^{n+1} - \Theta_i^n) \Delta z}{((q_w^{top})^{n+1} - (q_w^{bottom})^{n+1}) \Delta t} \quad (\text{Eq. 2-13})$$

An analogous mass balance ratio is defined for the air phase. A mass balance ratio of 1 is achieved by a mass-conserving numerical scheme. Celia et al (1990) pointed out that the mixed form of the equation is perfectly mass conservative. When the

2-3. Numerical results in one dimension

discrete versions of equation (Eq. 2-10) are summed over all the nodes of the domain, the interior flux terms cancel and the mass balance statement (Eq. 2-13) is attained. Celia et al. (1990) did not include the water storage term in their approximation. In this work the water storage term is included and it does contribute some mass balance errors. These mass balance errors are much less than 1% in the unsaturated zone as will be demonstrated in some of the examples in later sections.

2-2-6. Calculation of mass flux

The mass flux is calculated from the pressure solution for particle tracking purposes and for the contaminant transport solution. The mass flux is calculated at the center of each element from the fluid pressures using a centered difference approximation of Darcy's law (Eq. 1-6):

$$q_{\alpha_{i+1/2}}^{n+1} = -K_{\alpha_{i+1/2}}^{n+1} \left(\frac{H_{\alpha_{i+1}}^{n+1} - H_{\alpha_i}^{n+1}}{\Delta z} - \frac{\rho_{\alpha_{i+1/2}}^{n+1}}{\rho_{0w}} \sin \psi \right)$$

2-3. Numerical results in one dimension

The algorithm presented above has been used to solve a variety of one-dimensional, two-phase flow problems. Results are presented in this section to verify the behavior of the algorithm, to compare the numerical performance of this algorithm to others reported in the literature, and to examine certain physical phenomena of interest. To verify the algorithm and to examine details of air-phase flow under water infiltration, the experiments and associated numerical simulations of Touma and Vauclin (1986) are used. For comparison a finite element approximation to the traditional "h-based" form of the governing equations (Kaluarchchi and Parker, 1989), is also used to solve the examples of Touma and Vauclin (1986). These results are compared to those using the formulation presented above, with an emphasis on mass balance and on applicability of the schemes for more general two-phase problems. All the results reported below were generated using the code described in Appendix A. Additional cases can be considered by varying the initial and boundary conditions which can be easily input into the code.

2-3-1. Verification of numerical scheme

The first results are meant to test the model by comparison to published solutions for two-phase air-water systems. To this end, several problems reported in Touma and Vauclin (1986) were solved using the lumped finite element/modified Picard algorithm described above. These include both constant flux and constant head boundary conditions. All are one-dimensional and transient. The appropriate functional relationships for moisture content and relative permeability for water and air are (Eq. 1-8), (Eq. 1-13), (Eq. 1-14) respectively. They are illustrated in Figure 1-1.

An example of one of these simulations is a situation that involves a hydrostatic initial condition with water applied to the top boundary at the prescribed flux rate of 20 cm/h. The column is sealed at the bottom so that neither air nor water can escape, and the air is initially set to be at atmospheric pressure at the surface. In this case the flux of water at the top of the column exceeds K_{ws} , so that the water content continues to build up at the top of the column until $\theta_w = \theta_{ws}$. The time at which this occurs corresponds to the time at which the capillary pressure equals zero, and is defined as the ponding time t_p . At that time, air is at residual saturation at the top of the column, so that air cannot escape from the column. The air then builds up pressure until the capillary head reaches a critical value, defined by $h_{crit} = h_{ae}$ cm, where h_{ae} is the air entry pressure, or bubbling pressure, estimated by Touma and Vauclin (1986) as $h_{ae} = 14$ cm. At this point the air pressure head is defined so that the capillary pressure head is equal to 14 cm. The water content at the surface is then reduced to less than the maximum value on the imbibition curve; based on the results in Touma and Vauclin (1986), the water content is reduced to the value on the secondary imbibition curve corresponding to $h_c = 14$ cm. This allows air to escape to the surface. The water head at the surface after ponding is defined by the ponding depth, equal to the difference between the total flux applied and the total amount infil-

trated into the column. A schematic of the problem is illustrated in Figure 2-2, and relevant information is given in Table 2-1 (Example 3).

Table 2-1 *Boundary conditions for the experiments of Touma and Vauclin (1986).*

Example	Top Boundary Conditions	Bottom Boundary Conditions
Open Column		
1	$q_w = 8.3 \text{ cm h}^{-1}$ $h_a = 0.0$	$h_w = -9.9$ $h_a = 0.1204$
Bounded Column		
2	$q_w = 8.3 \text{ cm h}^{-1}$ $h_a = 0.0$	$q_w = 0.0$ $q_a = 0.0$
3	$q_w = 20 \text{ cm h}^{-1}$ for $0 \leq t \leq t_p$ $h_a = 0.0$ $h_w = 20 t - I(t)$ for $t_p < t \leq t_c$ $q_a = 0.0$ $h_w = 20 t - I(t)$ for $t > t_c$ $h_a = h_{ae} + h_w$	$q_w = 0.0$ $q_a = 0.0$

This problem is a good test of a two-phase simulator as it involves combinations of both fixed head and flux boundary conditions and, as Touma and Vauclin (1986) have shown, this is a case where the air phase has a significant retarding effect on the water movement. Numerical results showing moisture content profiles for several different times are shown in Figure 2-3. For comparison, numerical results of Touma and Vauclin (1986) are also shown. Satisfactory agreement is achieved. Similar agreement was obtained for all other test problems presented by Touma and Vauclin.

In this simulation and in each of the simulations discussed below we have used variable time stepping with an initial $\Delta t = 1$ second. The time step size was increased whenever the nonlinear iteration scheme converged in less than 10 iterations; Δt was decreased whenever the number of iterations was greater than 15. The error tolerance on the residual was $1 \times 10^{-6} \text{ sec}^{-1}$. For example, in the first problem discussed below, Δt increased from 1 sec. to approximately 32 sec. over the total simulation time. The column was discretized by using 101 nodes, which is equivalent to 100 elements. This corresponds to $\Delta z = 1 \text{ cm}$.

2-3-2. Air phase velocities

The paper of Touma and Vauclin (1986) addresses the question of when Richards equation is applicable. That is to say, under what conditions does the air phase behavior substantially alter the flow of water. Their answer, based on laboratory column experiments and subsequent numerical simulations, was that the air can significantly retard the motion of water only when air is trapped inside the soil column, that is when:

- (1) The top of the column is saturated or nearly so, and
- (2) the sides of the column are impervious, and
- (3) the bottom of the column does not allow air to escape.

Under this combination of conditions, the air phase has a significant influence on the infiltrating water. Otherwise when there is a path for the air to escape, it has sufficiently large mobility that it usually equilibrates quickly to (close to) atmospheric pressure. Thus Richards equation is usually a good approximation for describing the water phase motion under most transient water movement episodes.

Boundary Conditions for infiltration into a bounded column

Figure 2-2 Experimental setup for Example 3 of Table 2-1 showing boundary conditions before and after ponding occurs. Darker shading indicates higher water content.

Figure 2-3 Time evolution of moisture content profile comparing the numerical results with those of Touma and Vauclin (1986). (Note that the results of Touma and Vauclin depicted here are an approximate representation of the figure in their paper).

2-3. Numerical results in one dimension

However, applicability of Richards equation does not mean that the air phase is unimportant. Indeed, Richards equation depends on the air moving in whatever ways are necessary to "get out of the way" of the invading water (or to replace draining water). Under transient water infiltration or drainage, the air phase is never static. It is common to read statements such as:

"Unsaturated flow... is nothing but a special case of simultaneous flow of two immiscible fluids, where the non-wetting fluid (air) is assumed to be stagnant." (Bear 1988 pg. 474, see also Bear 1979)

or

"Most of the time it is assumed that the air phase is *immobile* in unsaturated media, so only the movement in the water phase is calculated; the pressure in the air phase is equal to the atmospheric pressure, taken as zero" (Marsily 1986 from section entitled Unsaturated flow with immobile air phase.)

The three widely used texts cited here evoke the incorrect assumption about the air phase; the correct assumption is that the air-phase mobility is much greater than the water-phase mobility so that the air phase remains at essentially atmospheric pressure (see, for example, Hillel, 1980; Morel-Seytoux, 1973).

For considerations of water movement and associated changes in moisture content, the assumption of large air mobility, which implies $p_a \approx 0$, means that the air phase has essentially no effect on the solution of the equations for the water phase. However, if transport of volatile contaminants in the unsaturated zone becomes a consideration, then the air-phase mobility may become quite important. Treatment of vapor phase transport as purely diffusive, which follows logically from the assumption of a static air phase, may be a poor assumption. In fact, when transient infiltration and/or drainage occurs, it should be expected that advective motion of both water and air phases might play a significant role in contaminant migration.

To demonstrate the motion of the air phase under different scenarios of water motion, a series of numerical experiments was performed based on the laboratory experiments of Touma and Vauclin. Instead of focusing on the transient moisture content distribution as was done by Touma and Vauclin (1986), air flow will be computed from the air pressures using Darcy's law. Three of the experiments are simulated here. The first allows both air and water to escape freely through the bottom of the column, while the second and third use a column that is bounded at the bottom so that neither fluid can escape. In the first and second cases, a flux of 8.3 cm/hr is applied, while a flux of 20 cm/hr is applied in the third case. The latter rate causes ponding while the former does not. Each these cases is outlined in Table 2-1.

2-3-3. Example 1. Open column, 8.3 cm/h flux rate

In the open column simulations, the air phase has been set to atmospheric pressure at both ends of the column. The water has a prescribed flux rate at the top of the column, in this case a flux of 8.3 cm/h which is less than the saturated hydraulic conductivity. The bottom condition for water is set to be -9.9 cm, which is equivalent to the condition given by Touma and Vauclin (1986). This allows air to escape through the bottom. The air boundary conditions are chosen so that without any infiltration into the column, the air is static because it is neutrally buoyant.

Figure 2-4 shows the infiltration of water and the movement of the air phase. Each vertical slice of the diagram is a snapshot of the column at a particular time. The grey scale is a measure of water content. At the left of the diagram is the grey scale for the initial hydrostatic water content, and as time increases, water can be seen infiltrating from the top of the column (which corresponds to the top of the diagram). The lines on the diagram are traces of particles of air as they are moved in the column. Initially, the particles are distributed according to the air content, so that more particles are placed where there is more air.

For a flux of 8.3 cm/h into the open column, the water can be seen to be infiltrating into the column and pushing the air ahead of the infiltration front downwards. As the water infiltrates, any air at or behind the front changes flow direction, and flows upward towards the surface. At the infiltration front there is a point where the air is stagnant, and the air moves away from this point both in an upwards and downwards direction. The physical explanation is that as the water infiltrates downwards, it increases the air pressure slightly in the vicinity of the infiltration front so that the air has a pressure gradient that drives flow towards both the top and the bottom of the column, allowing it to flow out both ends. This example is particularly interesting because it shows that even though there is a free path for the air to escape through the bottom of the column, some of the air still moves upwards, in the direction opposite to the water. Note that the slopes of the air particle traces give the velocity of the air, and that by counting the number of particle paths that pass through the top and bottom boundaries, relative volumes of air passing through each boundary can be estimated. In this case, approximately 36% of the air exiting the column in the first hundred minutes passes through the top of the column.

2-3-4. Example 2. Bounded column, 8.3cm/h flux

This example is the same as Example 1, except now the bottom of the column is sealed and does not allow either water or air to escape. The numerical results indicate that the air is essentially stagnant below the infiltrating front, while above

Figure 2-4 Time evolution of infiltrating water front (as shown in gray scale) and air movement (shown as particle trajectories) for Example 1: open column with a flux rate of 8.3 cmh^{-1} applied to the surface.

2-4. Two-dimensional numerical solution

the front the air moves quickly towards the surface. In this example air pressures build up significantly to allow the air to push its way through the water to the surface (Figure 2-5). This result is different from the result of Touma and Vauclin (1986), who predicted essentially no pressure build up. Our result appears to be reasonable as the flux of air out the top of the column must be essentially the same as the water going in but in an opposite direction to that of the water. That is, the flux of air out of the column must be approximately 8.3 cm/h; to achieve this flux with the high water saturations at the top of the column requires significant head gradients in the air phase. Despite the air pressure buildup in the column, the water still moves at velocities essentially equivalent to those in the open column, which also correspond to those associated with the Richards equation solution. This demonstrates that the build up of air pressure does not necessarily imply that the Richards approximation is not valid.

2-3-5. Example 3. Bounded column, 20cm/h flux

This column was described in detail above and is illustrated in Figure 2-2. In this case, despite the fact that the applied flux is significantly greater than in the previous examples, the water infiltrates at approximately the same rate as in Examples 1 and 2 (see Figure 2-6). In this case of ponding in a bounded column, air escapes out the top until ponding begins. After the onset of ponding, no air can escape until sufficient buildup of air pressure. When the capillary pressure reaches the entry pressure, air breaks through and the top boundary condition is set as $h_c = h_{ae} = 14$ cm. At this pressure, the water saturation is $\theta_w = 0.27$, and the associated water conductivity is approximately 6.4 cm/hr. This compares to a water conductivity of approximately 15.4 cm/hr when $\theta_w = \theta_{ws} = 0.312$, which would apply if the air did not break through at the top (for example in the case when the bottom of the column is open to air flow). Comparison of infiltration front velocities in the bounded versus open column cases, with an applied flux of 20 cm/hr, shows that in the open column the velocity is approximately twice as fast (during a 15 minute period the front in the bounded column moves approximately 10cm, while in the open column it moves approximately 20cm). A simple calculation shows that the reduction of infiltration velocity is essentially due to the reduction in conductivity:

$$\frac{K_{w_{top \text{ bounded}}}}{K_{w_{top \text{ open}}}} = \frac{6.4}{15.4} = 0.42 \approx \frac{10\text{cm}}{20\text{cm}} = \frac{\text{distance travelled in bounded column}}{\text{distance travelled in open column}}$$

This example demonstrates that the reduction of water-phase conductivity is largely responsible for the decrease in infiltration rate, not the air pressure build-up *per se*. This observation is consistent with the observations related to the pressure buildup in the previous example (Figure 2-5).

2-3-6. Numerical properties and comparison to head-based formulation

Mass balances associated with the results presented above show that even in the most computationally difficult case (bounded column with ponding), the maximum mass balance error in the air phase is 0.2%, while in the water phase it is 0.003% (see Figure 2-7). Air phase mass balance error is much better than 0.2% for most of the simulation, with the 0.2% error occurring during the time step in which the air breaks through at the top. Because the mass balance is calculated as mass accumulation divided by net influx through the top and bottom boundaries, the times between the onset of ponding and air break-through are not calculated (both numerator and denominator are zero).

These mass balance results can be compared to an analogous lumped finite element solution using the head-based form of the governing equations, wherein the time derivatives in (Eq. 2-1) and (Eq. 2-2) are written as

$$\frac{\partial \theta_w}{\partial t} = C_w \frac{\partial h_c}{\partial t}$$

and a standard Picard iteration is applied. Mass balance errors for this approximation were largest at early times (up to 33%). They also reached approximately 25% around the ponding time, and averaged about 5% at other times. These results are shown in Figure 2-7. Similar mass balance errors were reported by Kaluarachchi and Parker (1989) using a finite element approximation to the head based equations, applied to a two-liquid system. The reasons for these mass balance problems are the same as those discussed by Celia et al. (1990) in the context of Richards equation.

2-4. Two-dimensional numerical solution

The two-dimensional numerical solution of the air and water flow equations proceeds in an analogous way to the one-dimensional case. The relevant governing equations were given in section 1 ((Eq. 1-19) and (Eq. 1-20)):

Figure 2-5 Time evolution of air and water pressures (profiles plotted at 10 min intervals) for Example 2: bounded column with a flux rate of 8.3 cmh^{-1} applied to the surface.

Figure 2-6 Time evolution of infiltrating water front (as shown in gray scale) and air movement (shown as particle trajectories) for Example 3: bounded column with a flux rate of 20 cmh^{-1} applied to the surface.

Figure 2-7 Mass balance for air and water as a function of time, using the mixed form of the equations and using the head-based form of the equations.

2-4. Two-dimensional numerical solution

$$\begin{aligned}
 & \frac{\partial \theta_w}{\partial t} + S_{sw} \frac{\theta_w}{\phi} \frac{\partial h_w}{\partial t} - \frac{\partial}{\partial x} \left[K_{wx} \frac{\partial h_w}{\partial x} \right] - \frac{\partial}{\partial z} \left[K_{wz} \left(\frac{\partial h_w}{\partial z} - \sin \psi \right) \right] = F_w \\
 & (\phi - \theta_w) \frac{\rho_{0a}}{h_{0a}} \frac{\partial h_a}{\partial t} - \rho_a \frac{\partial \theta_w}{\partial t} \\
 & - \frac{\partial}{\partial x} \left[(\rho_a K_{ax}) \frac{\partial h_a}{\partial x} \right] - \frac{\partial}{\partial z} \left[(\rho_a K_{az}) \left(\frac{\partial h_a}{\partial z} - \frac{\rho_a}{\rho_{ow}} \sin \psi \right) \right] \\
 & = F_a
 \end{aligned}$$

Application of an Euler backward-in-time finite difference scheme and a modified Picard iteration scheme with a Taylor series expansion of $\Theta_w^{n+1, m+1}$ results in the equations:

$$\begin{aligned}
 & C_w^{n+1, m} \frac{\delta H_a^{n+1, m} - \delta H_w^{n+1, m}}{\Delta t} + S_{sw} \frac{\Theta_w^{n+1, m} \delta H_w^{n+1, m}}{\phi \Delta t} \\
 & - \frac{\partial}{\partial x} \left[K_{wx}^{n+1, m} \frac{\partial \delta H_w^{n+1, m}}{\partial x} \right] - \frac{\partial}{\partial z} \left[K_{wz}^{n+1, m} \frac{\partial \delta H_w^{n+1, m}}{\partial z} \right] \\
 & = - \frac{\Theta_w^{n+1, m} - \Theta_w^n}{\Delta t} - S_{sw} \frac{\Theta_w^{n+1, m} H_w^{n+1, m} - H_w^n}{\phi \Delta t} \\
 & + \frac{\partial}{\partial x} \left[K_{wx}^{n+1, m} \frac{\partial H_w^{n+1, m}}{\partial x} \right] + \frac{\partial}{\partial z} \left[K_{wz}^{n+1, m} \left(\frac{\partial H_w^{n+1, m}}{\partial z} - \sin \psi \right) \right] + F_w^{n+1} \\
 & \equiv R_w^{n+1, m}
 \end{aligned} \tag{Eq. 2-14}$$

and

$$\begin{aligned}
 & (\phi - \Theta_w^{n+1,m}) \frac{\rho_{0a} \delta H_a^{n+1,m}}{h_{0a} \Delta t} - \rho_a^{n+1,m} C_w^{n+1,m} \frac{\delta H_a^{n+1,m} - \delta H_w^{n+1,m}}{\Delta t} \\
 & - \frac{\partial}{\partial x} \left[(\rho_a K_{a_{xx}})^{n+1,m} \frac{\partial \delta H_a^{n+1,m}}{\partial x} \right] - \frac{\partial}{\partial z} \left[(\rho_a K_{a_{zz}})^{n+1,m} \frac{\partial \delta H_a^{n+1,m}}{\partial z} \right] \\
 & = \rho_a^{n+1,m} \frac{\Theta_w^{n+1,m} - \Theta_w^n}{\Delta t} - (\phi - \Theta_w^{n+1,m}) \frac{\rho_{0a} H_a^{n+1,m} - H_a^n}{h_{0a} \Delta t} \\
 & + \frac{\partial}{\partial x} \left[(\rho_a K_{a_{xx}})^{n+1,m} \frac{\partial H_a^{n+1,m}}{\partial x} \right] \\
 & + \frac{\partial}{\partial z} \left[(\rho_a K_{a_{zz}})^{n+1,m} \frac{\partial H_a^{n+1,m}}{\partial z} - \frac{(\rho_a^{n+1,m})^2}{\rho_{0w}} K_{a_{zz}}^{n+1,m} \sin \psi \right] \\
 & + F_a^{n+1} \\
 & \equiv R_a^{n+1,m}
 \end{aligned} \tag{Eq. 2-15}$$

Equations (Eq. 2-14) and (Eq. 2-15) are solved for $\delta H_\alpha^{n+1,m}$ ($\alpha = a, w$) at each iteration step as was done in the one-dimensional case. The equations are discretized in space using a Galerkin finite element scheme. The scheme is developed for the water equation here. The discretization of the air equation can be done in a similar way. The weak form of (Eq. 2-14) is written:

$$\begin{aligned}
 & \int_{\Omega} \left(C_w^{n+1,m} \frac{\delta H_a^{n+1,m} - \delta H_w^{n+1,m}}{\Delta t} + S_{sw} \frac{\Theta_w^{n+1,m} \delta H_w^{n+1,m}}{\phi \Delta t} \right) w \, d\Omega \\
 & - \int_{\Omega} \left(\frac{\partial}{\partial x} \left[K_w^{n+1,m} \frac{\partial \delta H_w^{n+1,m}}{\partial x} \right] + \frac{\partial}{\partial z} \left[K_w^{n+1,m} \frac{\partial \delta H_w^{n+1,m}}{\partial z} \right] \right) w \, d\Omega \\
 & = - \int_{\Omega} \left(\frac{\Theta_w^{n+1,m} - \Theta_w^n}{\Delta t} + S_{sw} \frac{\Theta_w^{n+1,m} H_w^{n+1,m} - H_w^n}{\phi \Delta t} \right) w \, d\Omega \\
 & + \int_{\Omega} \left(\frac{\partial}{\partial x} \left[K_w^{n+1,m} \frac{\partial H_w^{n+1,m}}{\partial x} \right] + \frac{\partial}{\partial z} \left[K_w^{n+1,m} \left(\frac{\partial H_w^{n+1,m}}{\partial z} - \sin \psi \right) \right] + F_w^{n+1} \right) w \, d\Omega
 \end{aligned}$$

for a given test function w .

The divergence of the flux in the above equation can be integrated by parts. This incorporates the boundary conditions into the formulation in a natural way. After the application of Green's theorem the resulting equations are:

$$\begin{aligned}
& \int_{\Omega} \left(C_w^{n+1,m} \frac{\delta H_a^{n+1,m} - \delta H_w^{n+1,m}}{\Delta t} + S_{sw} \frac{\Theta_w^{n+1,m} \delta H_w^{n+1,m}}{\phi \Delta t} \right) w \, d\Omega \\
& + \int_{\Omega} \left(\left[K_{wx}^{n+1,m} \frac{\partial \delta H_w^{n+1,m}}{\partial x} \right] \frac{\partial w}{\partial x} + \left[K_{wz}^{n+1,m} \frac{\partial \delta H_w^{n+1,m}}{\partial z} \right] \frac{\partial w}{\partial z} \right) d\Omega \\
& = - \int_{\Omega} \left(\frac{\Theta_w^{n+1,m} - \Theta_w^n}{\Delta t} + S_{sw} \frac{\Theta_w^{n+1,m} H_w^{n+1,m} - H_w^n}{\phi \Delta t} \right) w \, d\Omega \\
& - \int_{\Omega} \left(\left[K_{wx}^{n+1,m} \frac{\partial H_w^{n+1,m}}{\partial x} \right] \frac{\partial w}{\partial x} + \left[K_{wz}^{n+1,m} \left(\frac{\partial H_w^{n+1,m}}{\partial z} - \sin \psi \right) \right] \frac{\partial w}{\partial z} \right) d\Omega \\
& + \int_{\partial\Omega} (q_w^{n+1} \cdot n|_{\partial\Omega}) w \, dS + \int_{\Omega} F_w^{n+1} w \, d\Omega
\end{aligned}$$

To define the trial and test functions the domain is discretized into rectangles of size $\Delta x_i = x_{i+1} - x_i$ in the horizontal direction and $\Delta z_i = z_{i+1} - z_i$ in the vertical direction. The resulting discretization has E elements and N nodes.

Bases for the trial and test spaces are chosen to be the set of bilinear basis functions defined on the rectangular elements. The numerical formulation is analogous to that of Section 2-2-2, with the change being from one dimension to two dimensions. See Binning (1994) for details about specific elemental matrices and matrix assembly procedures.

2-4-1. Time lumping

The time lumping scheme used is the $L2$ scheme of Milly (1985). The $L2$ scheme lumps all the time coefficients onto the diagonal of the matrix. The $L2$ scheme was found to perform better than the $L1$ formulation which lumps the final coefficient of $\delta H_{w_i}^{n+1,m+1}$ onto the diagonal, but uses a distributed evaluation of the non-linear coefficients. Using this scheme the temporal integrals of the form:

$$\sum_{j=1}^N \frac{\delta H_{w_j}^{n+1,m+1}}{\Delta t} \int_{\Omega_i} \hat{C}_w \phi_j \phi_i \, dz$$

(where $\hat{C}_w$ is the numerical approximation to C_w) are replaced with:

$$\frac{\delta H_{w_i}^{n+1,m+1}}{\Delta t} C_{w_i}^{n+1,m} \int_{\Omega_i} \phi_i \, dz$$

The other temporal terms are treated in the same way. Bouloutas (1988) demonstrated that temporal lumping was an effective means of controlling finite element oscillations in the Richards equation in two dimensions.

2-4-2. Source/Sink terms

Source sink terms were described in the element equations by the term $\int_{\Omega_e} F_w^{n+1} \phi_i d\Omega$. Source/sink terms are

incorporated after the assembly of the global approximation. Source/sink terms are described by:

$$F_w^{n+1} = \sum_{j=1}^{No \text{ of wells}} Q_{w_j}^{n+1} \delta(x - x_j) \delta(z - z_j)$$

where the subscript j indexes the wells located at the nodes (x_j, z_j) and $\delta(z - z_j)$ is the delta function located at the node j . With this definition, the source/sink terms appear in the global approximation through:

$$\int_{\Omega} F_w^{n+1} \phi_i d\Omega = \begin{cases} Q_{w_i} & i = \text{well} \\ 0 & \text{otherwise} \end{cases}$$

2-4-3. Boundary conditions

When the global finite element approximation is found by summing the element equations, the boundary terms arising

in the integrals $\int_{\partial\Omega_e} q_w \cdot n |_{\partial\Omega_e} \phi_i dS$ must be evaluated. Two types of boundary condition are considered. For a

Dirichlet, or fixed head boundary condition, the finite element equation at boundary node i is replaced with the statement that:

$$\delta H_{\alpha_i}^{n+1, m} = 0, \quad H_{\alpha_i}^{n+1} = \text{given}.$$

The other form of boundary condition is a second-type or specified fluid flux condition. A flux boundary condition is incorporated into the assembled or global approximation at boundary node i through:

$$\int_{\partial\Omega_e} q_w \cdot n |_{\partial\Omega_e} \phi_i dS = \frac{q_{n1} l_1}{2} + \frac{q_{n2} l_2}{2}$$

where q_{n1}, q_{n2} are the specified fluid fluxes through the boundary of the elements of length l_1, l_2 adjacent to node i .

2-4-4. Air equation

The finite element approximation to the air equation is similar to that of the water equation. It should be noted, however, that the nonlinear coefficients in the air equation are approximated through:

$$\rho_a(h_a) K_{a_{zz}}(h_c) \approx \sum_{j=1}^E (\rho_{a_j} K_{w_{zz_j}}) \phi_j(x, z)$$

$$\rho_a^2(h_a) K_{a_{zz}}(h_c) \approx \sum_{j=1}^E (\rho_{a_j}^2 K_{w_{zz_j}}) \phi_j(x, z)$$

2-5. Verification of code and example problems

The code was verified by comparison with the one-dimensional two-phase code for a one-dimensional problem. The boundary conditions are illustrated in Figure 2-8. The pressure field from each of the two codes is shown in Figure 2-9. The small differences between the one- and two-dimensional solutions that can be observed in the figure that are caused by minor differences in the implementation of the finite elements.

Once the code has been verified against the one-dimensional code, it can be used to study two-dimensional problems. The first two-dimensional example is that of infiltration from a strip source into an initially dry uniform Touma and Vauclin (1986) coarse sand. The boundary conditions, initial conditions and the discretization used for this simulation are illustrated in Figure 2-10.

Variable time step sizes were used to solve this problem. Initially, when the infiltrating pressure front is steep, the nonlinearities are strong and a small time step must be chosen. In this case the initial time step size was 100 seconds. As time passes the infiltrating front smooths and the nonlinearities weaken. This can be seen as the Picard iteration scheme requires fewer iterations to converge as time passes. As the amount of iterations decreases below 5 for the current time step, the time step size is increased by a factor of 1.05. The final time step size for this simulation was 167 seconds. The amount of time-step acceleration possible for this two-dimensional problem is small compared to those observed in the one-dimensional simulations. In two dimensions it was possible to achieve an increase of only 167% of the initial time step. In one dimension for example problem 3 of Table 2-1 it was possible to increase the time-step from an initial size of 1 second to 37 seconds. In the two-dimensional examples the smaller threshold of 5 before time step size can be increased, reflects the more difficult nature of two-dimensional problems. With the Picard iteration scheme, there is always a tradeoff between the number of iterations and the size of time step that can be taken, with larger time steps generally requiring more iterations.

The flow of air and water are shown in Figure 2-11. The gray scale in Figure 2-11 shows the distribution of water at time 25 hours. The darker shades indicate higher moisture contents and the lighter shades lower moisture contents. The paths of the air are shown by arrows on the figure. Each arrow represents the trajectory of an air particle over a 25-hour period. The figure shows the expected bulb-like infiltration of water into the unsaturated zone with capillary diffusion in the vertical and horizontal directions. The air paths radiate outwards from the water, illustrating that the air moves out of the path of the infiltrating water. Interestingly, with the water moving downwards and the air free to escape through all sides of the transect, it moves upwards and sideways towards the boundary as well as downwards toward the bottom. This result was predicted in one dimension when example problems were discussed for column experiments with both ends of the column open to the air. In these examples, there is a slight pressure increase in front of the infiltrating water which causes a pressure gradient to occur to all the boundaries of the domain that are open to the air phase. The air then moves both sideways and upwards as well as downwards to move out of the way of the infiltrating water.

A second example considers the effect of heterogeneity on the flow of air and water by embedding loam lenses into the homogeneous sand of Figure 2-10. The lenses are a hypothetical loam with properties described by the van Genuchten pressure saturation relation (Eq. 1-8) with parameters:

$$\begin{aligned}\theta_{ws} &= 0.35 \text{ cm}^3/\text{cm}^3; & \theta_{wr} &= 0.1 \text{ cm}^3/\text{cm}^3 \\ \alpha &= 0.034 \text{ cm}^{-1} & n &= 3.2\end{aligned}$$

and the Mualem theory conductivity functions specified by (Eq. 1-8), (Eq. 1-11) and (Eq. 1-12) with:

$$K_{ws} = 1.512 \text{ cm/h}$$

$$K_{as} = \frac{\mu_w}{\mu_a} K_{ws} = 279 \text{ cm/h}$$

where relation (Eq. 1-5) was used to derive the equation $K_{as} = \frac{\mu_w}{\mu_a} K_{ws}$. The pressure saturation curves for the sand and

loam are shown in Figure 2-12. The sand matrix is Touma and Vauclin sand with the properties described in section 1.

The distribution of the loam lenses is illustrated in Figure 2-13. The flow of air and water at time 25 hours is shown in Figure 2-11. In this example the loam lenses are essentially impermeable units embedded in the coarse sand matrix. The water and air flow around the lenses rather than through them. For example, rather than flowing through lenses 2 and 4 the water flows on top of the lenses and around them. Additional examples of heterogeneous systems, including simulations related to the field experiments at the USGS Cape Cod Research Site, can be found in Binning (1994).

Initial Conditions $h_w = -100\text{cm}$, $h_a = \text{'air static'}$ (linear from top to bottom)

Figure 2-8 Boundary conditions for the comparison of the one-dimensional and two-dimensional two-phase flow codes.

Figure 2-9 Comparison of one- and two-dimensional two-phase flow codes for the boundary and initial conditions illustrated in Figure 2-8 and different discretization sizes.

All water boundaries no flow except at strip source

Initial conditions:

$h_w = -100$ cm,

h_a varies linearly with height between

$h_a = 0$ at top and $h_a = 0.1204$ at bottom.

Figure 2-10 Material distribution, boundary and initial conditions for infiltration from a strip source into a uniform initially dry transect of coarse Touma and Vauclin (1986) sand.

Figure 2-11 Flow solution for infiltration into a uniform coarse Tournai and Vauclain (1986) sand. The figure shows the water infiltration in gray scale and has superposed the paths of particles of air.

Figure 2-12 *Pressure-saturation curves for the coarse sand of Touma and Vauclin (1986) and a hypothetical loam.*

All water boundaries no flow except at strip source

Initial conditions:

$h_w = -100$ cm,

h_a varies linearly with height between

$h_a = 0$ cm at top and $h_a = 1.204$ cm at bottom.

Materials

Sand

Loam

Figure 2-13 Material distribution, boundary and initial conditions for infiltration from a strip source into a transect of coarse Touma and Vauclin (1986) sand embedded with loam lenses. The numbering of the lenses is used in the discussion in the text.

Figure 2-14 Flow solution for infiltration into a coarse Touma and Vauclin (1986) sand embedded with loam lenses at time 25 hours. The distribution of the lenses is shown in Figure 2-13.

In the context of remediation of a volatile organic compound, heterogeneities may play a significant role. It could be envisaged that large amounts of a volatile organic contaminant may be found embedded in the loam lenses. Yet when air is pumped through the unsaturated zone in a contaminant to remediate it in a venting scheme, the air is likely to flow around the lenses and avoid the contaminant. In practice, it is observed at venting sites that when the venting scheme is in operation the contaminant concentration decreases. After the pump is turned off the contaminant concentration in the air phase is often observed to recover. This could be because the contaminant that is removed by the venting operation is predominantly in the high permeability units. When the air pumping is halted, the volatile contaminant diffuses from the low permeability units back into the high permeability materials, increasing the concentration there.

There is a large contrast between the material heterogeneities considered in the above hypothetical example. In many natural porous materials there is less contrast between materials.

2-6. Discussion

The numerical methods used in this section lead to robust and reliable solutions to the coupled set of nonlinear equations that describe the simultaneous movement of water and air in unsaturated soils. The methods use extensions of the Modified Picard method developed previously for Richards' equation (Celia et al., 1990). The code developed for this work allows for general boundary conditions and for general variability of material properties. Documentation for the one-dimensional version of the code is provided as Appendix A.

The examples presented in this section demonstrate physical behaviors of the water and air phases under short-time forcings, in this case infiltration. The examples based on the laboratory experiments of Touma and Vauclin (1986) demonstrate that the air-phase is highly dynamic, and that the common assumption of a static air phase is incorrect. This is true for any infiltration problem, independent of the applicability of Richards' assumption. The two-dimensional results corroborate the observations associated with the one-dimensional examples. The two-dimensional example with material heterogeneities demonstrates the ability of the algorithm to accommodate heterogeneous materials. The implications of heterogeneities are wide-ranging, as the further discussions in Binning (1994) demonstrate.

The model problems presented herein appear to be representative of typical short-time dynamic responses of unsaturated systems to infiltration events. Additional factors that may be important, and that can be incorporated easily into the code described herein, include barometric pumping (a time-varying boundary condition for air pressure at the land surface) and variable rainfall rates (a time-varying boundary condition for water flux at the land surface).

Other numerical approaches may be used to solve this set of equations. Of particular interest is the so-called global pressure - fractional flow approach. In this approach, the two phase-equations are combined and rewritten so that one equation has a non-linear elliptic form and the second has a non-linear advection-diffusion form. There are several distinct advantages to using this form of the equations. First, characteristic-type methods may be used to solve the non-linear advection-diffusion equation. This allows much larger time steps to be used, leading to numerical solutions that are much more computationally efficient. Details about this type of approach may be found in Celia and Binning (1992b) and in Binning (1994). At this point, the main drawback of the approach is that it is not amenable to general boundary conditions, due to the different combinations of terms that appear in the equations. There are also unresolved questions regarding incorporation of general material heterogeneities. While we have formulations that address these deficiencies, they have yet to be implemented. Therefore, at this point, the so-called two-pressure approach is preferred. Despite the significant computational requirements associated with this method, its robustness and relative ease of implementation in multi-dimensional problems are strong benefits of the method.

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3. *Solution of the transport equations by finite elements*

3-1. *Introduction*

The transport of pollutants in the unsaturated zone is modelled using two sets of equations. The first set of equations describes the pressure, saturation, and volumetric flux in each of the fluid phases. These equations have been solved in the preceding sections. The second set of equations describes the way that each of the fluid phases transports a miscible contaminant. The physical processes associated with pollutant transport were described mathematically in section 1. In this work it is assumed that the flow processes do not depend on the transport processes. This enables us to solve the flow equations independently of the transport equations. However, the transport processes require the definition of the flow fields and so the logical sequence is to first solve the flow equations and then solve the transport equations.

In the literature of recent years there has been a profusion of studies of the transport equations in the unsaturated zone. The impetus for this rapid development has been the strict regulatory stance on ground-water pollution initiated in the mid 1980's (Gee et al. 1991). Since that time, research on contamination in the unsaturated zone has evolved dramatically resulting in a corresponding increase in numerical models available. Each model has different features that tailor the model to the particular application for which it was designed. The models use a variety of solution techniques. These include: analytical solutions, finite difference, finite element, particle tracking and Eulerian-Lagrangian methods. Ong et al. (1992) summarized the available models and their features. Table 3-1 is a similar table to that of Ong et al. (1992). It includes recent references, some additional features and groups the models according to the method of solution. While the models differ greatly in their available features, the models using similar solution technique will have similar numerical behavior. The contaminant transport models that are discussed here specifically include a gas phase. There are many other more general multiphase transport models available that could be applied to the problem of unsaturated zone contaminant transport. A survey of these models is available in the comprehensive review papers of Miller et al. (1991) and Mayer et al. (1992).

Analytical models are typically used in restrictive settings such as for modelling transport in experimental column studies with homogeneous materials (Shoemaker et al. 1990, Jury et al. 1983), to test the accuracy of numerical approximations to the equations (for example T.C. Yeh et al. (1993)), and as simple but powerful diagnostic tools for evaluation of field sites (Johnson 1990a, 1992). In these settings the exact solution of the governing equations is possible and the models have been applied quite successfully Johnson (1990b). However, for more complex geometries, boundary conditions, and heterogeneous materials, numerical solutions must be sought.

Finite difference techniques are the simplest of the numerical techniques to apply and there is a large number of models using this solution technique. Weeks et al. (1982) were some of the first to use a numerical model to study transport in the unsaturated zone. The finite difference models range from the simple one-dimensional model of Rosenbloom (1993), through to the comprehensive model of Sleep and Sykes (1993). The finite difference models have used forward Euler (explicit) time stepping (Benson et al. 1993), variably weighted Euler (Crank-Nicholson) time stepping (Baehr and Corapcioglu 1987) or backward Euler (fully implicit) time stepping [Sleep and Sykes (1993), Rathfelder (1991)].

Sleep and Sykes (1993) present an excellent summary of the arguments for the different forms of temporal discretization. The implicit method is more computationally expensive than the explicit method. The implicit time stepping scheme is unconditionally stable, so that large time steps can be taken. However, large time steps may not be advantageous in an implicit scheme as the truncation error increases with time step size leading to a loss of accuracy in the solution. The implicit scheme also adds more numerical diffusion to the solution than the explicit method. In contrast, the explicit methods do have a limitation on the time step size, so that small time steps must be taken. Accuracy of an explicit scheme increases with increasing time step size. These and other arguments summarized by Sleep and Sykes (1993) illustrate that there are many arguments for and against each method and that the choice of temporal discretization is a difficult one.

Another common numerical approach to solving the transport equations has been to use the finite element method. Galerkin finite element methods were applied by Mohsen et al. (1980), Metcalf and Farquhar (1987), Dorgarten (1989), Mendoza and Frind (1990), and Culver et al. (1991). The deficiencies of the finite element method for solving the transport equation are well known. The solutions obtained by the method are prone to oscillations and contain significant numerical diffusion. Several researchers have tried to improve the finite element solution by adding upstream weighting. Upstream weighting was demonstrated to be effective in reducing oscillations in the saturated transport equation by Heinrich et al. (1977) and Dick (1983). Bouloutas (1989) applied upstream weighting for transport in the water phase in the unsaturated zone. He demonstrated that upstream weighting could be effectively employed to reduce oscillation, while not adding significant numerical diffusion.

Table 3-1 Summary of available vapor-phase flow and transport models.

References	Features															
	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
Jury et al., 1983	A	1			x		x	x	x	x		x				
Johnson, 1991	A	2	x	x	x	x									x	
Shoemaker et al., 1990	A	2			x		x	x	x	x		x				
Weeks et al., 1982	FD	1			x	x			x	x				x		
Abriola & Pinder, 1985	FD			x	x		x	x	x				x	x	x	x
Bear & Corapcioglu, 1987	FD	1		x	x		x	x	x	x		x		x	x	x
Rathfelder et al., 1991	FD	2	x	x	x	x			x	x	x				x	
Benson et al., 1993	FD	2		x	x	x			x					x		
Rosenbloom et al. '93	FD	1			x			x	x	x						
Sleep and Sykes, 1993	FD	3		x	x	x	x	x	x	x			x	x	x	x
Mohsen et al., 1980	FE	2	x		x	x								x		x
Metcalf & Farquhar, 1987	FE	2			x	x		x	x					x		x
Bouloutas 1989	FE	2					x	x						x		
Dorgarten, 1989	FE	2					x	x		x		x	x	x	x	
Mendoza & Frind, 1987	FE	2	x		x	x			x	x						x
Culver et al., 1991	FE	2			x		x	x	x	x			x	x		
McCarthy & Johnson, '93	R	2			x	x							x			
Yeh et al. 1993	EL	2					x	x		x			x	x		
Binning 1994	FE	2	x		x	x	x	x	x	x	x	x	x	x		
Binning 1994	EL	2			x	x	x	x	x	x			x	x		

1. Approximation type A-analytical FD-finite difference FE-finite element R-random walk EL-eulerian lagrangian 2. number of dimensions 3. radial geometry 4. multicomponent 5. diffusion, vapor phase 6. advection, vapor phase 7. diffusion, water phase 8. advection, water phase 9. dissolution (Henry's law) 10. sorption at solid liquid interface 11. non-equilibrium mass transfer 12. biodegradation/chemical reactions 13. coupled flow solution in both phases 14. heterogeneity 15. immiscible phase 16. density dependant on concentration

Recently, there have been several other approaches employed to solve the transport equations. These include the random walk method of McCarthy and Johnson (1993) which has the advantage of accurately representing the diffusive processes in the air phase. Both the finite element method and the finite difference method tend to overestimate the actual diffusion because of the addition of numerical diffusion to the solution.

Eulerian-Lagrangian techniques have also been popular for solution of the general single phase transport equation. These methods exploit the hyperbolic nature of the transport equations by using a characteristic type of formulation. Notable amongst recent applications of this technique is the work of Yeh et al. (1993) who applied the modified method of characteristics to water phase transport in the unsaturated zone.

The transport model discussed in this section is a finite element model. The features of this model are shown in the second-to-last row of Table 3-1. The last row of the table shows the features of the Eulerian-Lagrangian Localized Adjoint Method (ELLAM) model that is detailed in Binning (1994). From the table, it can be seen that the only other model that includes both the air and water phase with advective fluxes in both phases is the model of Sleep and Sykes (1993). This model is a finite difference model and does not include either reactions or kinetic phase transfer between the water and air phases. Both the finite element method and the finite difference method have numerical limitations that are well-known; these are overcome in the ELLAM. Simulations discussed in this section use the finite element solution with sufficiently fine discretization to avoid numerical problems.

The current section is divided into four parts. In the first part the transport equations with equilibrium mass transfer between the air and water phases are solved in one dimension and the finite element formulation discussed. In the second part the equations will be solved with a kinetic mass transfer between phases in one dimension. Next, the equilibrium case is discussed in two dimensions with a cartesian geometry. Finally the two-dimensional model is applied to the design of a low level radioactive waste disposal facility.

3-2. Equation formulation: Equilibrium case

The equation that will be solved in the first part of the section is the equilibrium transport equation. In section 1 this equation was derived and shown to have the form (Eq. 1-22):

$$\begin{aligned} & \frac{\partial ((R\theta_w + H\theta_a) c_w)}{\partial t} + \nabla \cdot ((q_w + Hq_a) c_w) - \\ & \nabla \cdot ((\theta_w D_w + \theta_a H D_a) \cdot \nabla c_w) + (\lambda_w \theta_w + H \lambda_a \theta_a) c_w \\ & = (F^w + F^a) \end{aligned} \quad (\text{Eq. 3-1})$$

In this section we will rewrite this equation using simpler notation as:

$$L(c) = \frac{\partial (\theta c)}{\partial t} + \nabla \cdot (qc) - \nabla \cdot (D \cdot \nabla c) + \lambda c = F \quad (\text{Eq. 3-2})$$

where:

$$\theta = (R\theta_w + H\theta_a)$$

$$q = (q_w + Hq_a)$$

$$D = \theta_w D_w + H\theta_a D_a$$

$$\lambda = \lambda_w \theta_w + H \lambda_a \theta_a$$

$$c = c_w$$

3-3. One-dimensional finite element solution

The equation is defined in the semi-infinite domain Ω_x , and is subject to the boundary conditions:

$$\begin{aligned} c(x, t) &= g_1(x, t) & (x \in \partial\Omega_x^1, t > 0) \\ (-D \nabla c(x, t)) \cdot n|_{\partial\Omega_x} &= g_2(x, t) & (x \in \partial\Omega_x^2, t > 0) \\ (qc(x, t) - D \cdot \nabla c(x, t)) \cdot n|_{\partial\Omega_x} &= g_3(x, t) & (x \in \partial\Omega_x^3, t > 0) \end{aligned} \quad (\text{Eq. 3-3})$$

Here the portion of the boundary of the spatial domain with boundary condition of type i is denoted $\partial\Omega_x^i$.

The initial conditions must also be specified and are of the form:

$$c(x, 0) = g_0(x) \quad x \in \Omega_x$$

3-3. One-dimensional finite element solution

In one dimension the governing equation is written:

$$\frac{\partial(\theta c)}{\partial t} + \frac{\partial(qc)}{\partial z} - \frac{\partial}{\partial z} \left(D \frac{\partial c}{\partial z} \right) + \lambda c = 0$$

where in one dimension source and sink terms will not be considered. The equation is discretized in time using a variably weighted difference scheme:

$$\begin{aligned} &\frac{(\theta c)^{n+1} - (\theta c)^n}{\Delta t} + \gamma \left[\frac{\partial(qc)}{\partial z} - \frac{\partial}{\partial z} \left(D \frac{\partial c}{\partial z} \right) + \lambda c \right]^{n+1} \\ &(1 - \gamma) \left[\frac{\partial(qc)}{\partial z} - \frac{\partial}{\partial z} \left(D \frac{\partial c}{\partial z} \right) + \lambda c \right]^n \\ &= 0 \end{aligned} \quad (\text{Eq. 3-4})$$

The scheme is fully implicit with $\gamma = 1$, and explicit with $\gamma = 0$.

A Galerkin finite element scheme is applied to the spatial terms. First the weak form of (Eq. 3-4) is found by introducing the test function $w(z)$ and integrating the equation over the spatial domain $(0, l)$:

$$\begin{aligned} &\int_0^l \left\{ \frac{(\theta c)^{n+1} - (\theta c)^n}{\Delta t} + \gamma \left[\frac{\partial(qc)}{\partial z} - \frac{\partial}{\partial z} \left(D \frac{\partial c}{\partial z} \right) + \lambda c \right]^{n+1} \right. \\ &\quad \left. (1 - \gamma) \left[\frac{\partial(qc)}{\partial z} - \frac{\partial}{\partial z} \left(D \frac{\partial c}{\partial z} \right) + \lambda c \right]^n \right\} w \, dz \\ &= 0 \end{aligned}$$

The spatial derivatives in the equation are integrated by parts:

$$\int_0^l \left\{ \gamma \left(\frac{\partial (qc)}{\partial z} - \frac{\partial}{\partial z} \left(D \frac{\partial c}{\partial z} \right) \right)^{n+1} \right\} w \, dz$$

$$= \gamma \left[\left(qc - D \frac{\partial c}{\partial z} \right) w \right]_0^l - \gamma \int_0^l \left(qc - D \frac{\partial c}{\partial z} \right)^n \frac{dw}{dz} \, dz \quad (\text{Eq. 3-5})$$

In this equation it is convenient to integrate all the spatial derivatives by parts so that the sum of the advective and diffusive fluxes appears in the boundary term. It can be shown that applying Green's theorem to the advective term results in an equivalent approximation to the one obtained if Green's theorem is not used (Celia and Gray 1992).

The finite-dimensional solution space is defined by partitioning the domain into $N-1$ elements (z_1^e, z_2^e) , where z_1^e and z_2^e are the coordinates of the left and right coordinates of the element e . The trial and test functions are chosen to be the space of linear basis functions which are defined in local coordinates by:

$$\phi_1(\zeta) = \frac{1-\zeta}{2} \quad \phi_2(\zeta) = \frac{1+\zeta}{2}$$

where the local coordinate is related to the global coordinate system by:

$$\zeta = \frac{2z - (z_1^e + z_2^e)}{z_2^e - z_1^e}$$

These functions were illustrated in Figure 2-1.

Using these definitions of the basis functions, the concentration c is approximated:

$$c(z) \approx \sum_{j=1}^N c_j \phi_j(z)$$

and θc by:

$$\theta c \approx \sum_{j=1}^N \theta_j c_j \phi_j(z)$$

and the test function w is chosen from the set of linear basis functions $\phi_i(z)$. Finally the integrals over the domain are evaluated element wise so that:

$$\int_0^l dz = \sum_{e=1}^{N-1} \int_{z_1^e}^{z_2^e} dz$$

3-3. One-dimensional finite element solution

With these definitions the integrals can be evaluated in each element using the following:

$$\begin{aligned}
 & \sum_{j=1}^N \frac{\theta_j^{n+1} c_j^{n+1}}{\Delta t} A_{ij}^e - \gamma \left(q_e^{n+1} \sum_{j=1}^N c_j^{n+1} B_{ij}^e - D_e^{n+1} \sum_{j=1}^N c_j^{n+1} E_{ij}^e - \lambda \sum_{j=1}^N c_j^{n+1} A_{ij}^e \right) \\
 & + \left[\left(qc - D \frac{\partial c}{\partial z} \right)^{n+1} w \right]_{z_i^e}^{z_2^e} \\
 & = \sum_{j=1}^N \frac{\theta_j^n c_j^n}{\Delta t} A_{ij}^e + (1 - \gamma) \left(q_e^n \sum_{j=1}^N c_j^n B_{ij}^e - D_e^n \sum_{j=1}^N c_j^n E_{ij}^e - \lambda \sum_{j=1}^N c_j^n A_{ij}^e \right)
 \end{aligned} \tag{Eq. 3-6}$$

In equation (Eq. 3-6) the boundary terms are evaluated at the $n+1$ time level, the flux and dispersion are assumed spatially constant within each element, and the elemental integrals are given by:

$$A_{ij}^e = \int_{z_1^e}^{z_2^e} \phi_j \phi_i dz = (z_2^e - z_1^e) \begin{bmatrix} \frac{1}{3} & \frac{1}{6} \\ \frac{1}{6} & \frac{1}{3} \end{bmatrix}$$

$$B_{ij}^e = \int_{z_1^e}^{z_2^e} \phi_j \frac{\partial \phi_i}{\partial z} dz = \begin{bmatrix} -\frac{1}{2} & -\frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{bmatrix}$$

$$E_{ij}^e = \int_{z_1^e}^{z_2^e} \frac{\partial \phi_j}{\partial z} \frac{\partial \phi_i}{\partial z} dz = \frac{1}{(z_2^e - z_1^e)} \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}$$

When the element equations are assembled the boundary terms $\left[\left(qc - D \frac{\partial c}{\partial z} \right)^{n+1} w \right]_{z_i^e}^{z_2^e}$ cancel on interior boundaries. The

assembled equation at an interior node i is written:

$$\begin{aligned}
 & \frac{1}{\Delta t} \left(\frac{1}{6} \theta_{j-1}^{n+1} c_{j-1}^{n+1} + \frac{2}{3} \theta_j^{n+1} c_j^{n+1} + \frac{1}{6} \theta_{j+1}^{n+1} c_{j+1}^{n+1} \right) \\
 & + \gamma \left(q_{i+\frac{1}{2}}^{n+1} \frac{c_{i+1}^{n+1} + c_i^{n+1}}{2\Delta z} - q_{i-\frac{1}{2}}^{n+1} \frac{c_i^{n+1} + c_{i-1}^{n+1}}{2\Delta z} \right) \\
 & - \gamma \left(D_{i+\frac{1}{2}}^{n+1} \frac{c_{i+1}^{n+1} - c_i^{n+1}}{\Delta z^2} - D_{i-\frac{1}{2}}^{n+1} \frac{c_i^{n+1} - c_{i-1}^{n+1}}{\Delta z^2} \right) \\
 & + \gamma \lambda \left(\frac{1}{6} c_{j-1}^{n+1} + \frac{2}{3} c_j^{n+1} + \frac{1}{6} c_{j+1}^{n+1} \right) \\
 & = \frac{1}{\Delta t} \left(\frac{1}{6} \theta_{j-1}^n c_{j-1}^n + \frac{2}{3} \theta_j^n c_j^n + \frac{1}{6} \theta_{j+1}^n c_{j+1}^n \right) \\
 & - (1-\gamma) \left(q_{i+\frac{1}{2}}^n \frac{c_{i+1}^n + c_i^n}{2\Delta z} - q_{i-\frac{1}{2}}^n \frac{c_i^n + c_{i-1}^n}{2\Delta z} \right) \\
 & + (1-\gamma) \left(D_{i+\frac{1}{2}}^n \frac{c_{i+1}^n - c_i^n}{\Delta z^2} - D_{i-\frac{1}{2}}^n \frac{c_i^n - c_{i-1}^n}{\Delta z^2} \right) \\
 & - (1-\gamma) \lambda \left(\frac{1}{6} c_{j-1}^n + \frac{2}{3} c_j^n + \frac{1}{6} c_{j+1}^n \right)
 \end{aligned}$$

Boundary conditions are specified at node 1 and node N . If the concentration is given, the equation is replaced by the statement of the boundary condition. If the total flux $(qc - D \frac{\partial c}{\partial z})$ is given, it is placed on the right hand side of the above equation. For a second type boundary condition of a prescribed concentration gradient, the known boundary concentration gradient is placed on the right hand side of the equation while the unknown boundary advective flux is placed on the left side of the equation.

3-3-1. Numerical behavior of the solution

The numerical behavior of the finite element method for the transport equation is well known in one dimension (see for example Daus et al. 1985). In order that accurate solutions are obtained, several guides on the discretization should be followed. The Courant number:

$$Cr = \frac{v\Delta t}{\Delta z} \quad (\text{Eq. 3-7})$$

should be chosen so that $Cr \leq 1$ in order that the equation satisfies the CFL (Courant, Friedrichs, Levy, 1928) condition. The Peclet number:

$$Pe = \frac{v\Delta x}{D}$$

which measures the ratio between advective and diffusive flux should be chosen so that $Pe \leq 2$. Daus et al. (1985) use numerical experiments to demonstrate the behavior of the finite element method in cases where the Peclet and Courant number criteria are not met. They show that if the Peclet and Courant number criteria are not met there are no general rules for predicting the solution behavior.

3-3-2. Lumping

Daus et al. also studied the effectiveness of mass lumping for the finite element discretization of the transport equation. Lumping of the temporal terms is accomplished by diagonalizing the matrix A_{ij} , so that:

3-4. Kinetic mass transfer in one dimension

$$A_{ij}^e = \frac{(z_2^e - z_1^e)}{2} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

Daus et al. (1985), among others, have shown that in one dimension the consistent formulation of the temporal term has less numerical error than the lumped formulation. The analysis of Daus et al. (1985) is based on numerical experiments. A more rigorous approach is to use Fourier analysis to examine the oscillatory behavior. Such an approach is outlined in Pinder and Gray (1977), Celia and Gray (1992), and Binning (1994). These analyses show why lumping is less effective in one dimension than in higher dimensions.

3-3-3. Time weighting

A number of authors have used the Crank-Nicholson difference scheme (see Table 3-1) in preference to a fully implicit formulation. The Crank-Nicholson scheme adds less numerical diffusion to the approximation as can be demonstrated with a simple truncation error analysis. While this strategy may seem beneficial in one dimension, the added numerical diffusion of a fully implicit scheme is desirable in multiple dimensions to control oscillations. Unless otherwise stated the numerical solutions presented herein use the Euler backward difference scheme in time.

3-4. Kinetic mass transfer in one dimension

The equations used to model kinetic mass transfer were derived in section 1. In one dimension (Eq. 1-24) can be written:

$$\begin{aligned} \frac{\partial(\theta_w c_w)}{\partial t} + \frac{\partial(q_w c_w)}{\partial z} - \frac{\partial}{\partial z}(\theta_w D_w \frac{\partial c_w}{\partial z}) + \lambda_w \theta_w c_w &= K \theta_a (c_a - H c_w) \\ \frac{\partial(\theta_a c_a)}{\partial t} + \frac{\partial(q_a c_a)}{\partial z} - \frac{\partial}{\partial z}(\theta_a D_a \frac{\partial c_a}{\partial z}) + \lambda_a \theta_a c_a &= -K \theta_a (c_a - H c_w) \end{aligned} \quad (\text{Eq. 3-8})$$

The finite element discretization of (Eq. 3-8) proceeds in a manner analogous to that described above for the equilibrium case. The right hand side terms accounting for the mass transfer between phases are treated in the same way as the reaction terms. The only additional difficulty is the coupling of the transport equation for the water and air phases through the right hand side terms. This means that the two transport equations must be solved simultaneously. In the equilibrium case, the equation at node i involved the concentration at nodes $i-1$, i , $i+1$. The resultant matrix was tridiagonal. For the nonequilibrium case, the equation at node i for phase α involves the concentration in phase α at nodes $i-1$, i , $i+1$, and the concentration in the other phase at node i . By arranging the equations for the air and water phases so that the air equation at node i follows the water equation at node i the system of equations can be seen to have a pentadiagonal structure.

The effect of the non-equilibrium phase partitioning is examined by studying the path of a TCE contaminant that is initially dissolved in the water phase at 30cm depth in a 100cm long column filled with Touma and Vauclin (1986) coarse sand. The column and flow conditions were described in section 2, Table 2-1. A water infiltration rate of 20cm/hr is imposed at the surface. The water ponds on the surface and the air, whose only path of escape is through the top of the column, bubbles through the top of the column. The flow of each of the two phases is illustrated in Figure 3-1. In the figure it can be seen that the air is moving up while the water moves down.

The contaminant transport is studied under three scenarios. Either the contaminant moves only in the water phase, it moves in both phases with equilibrium phase partitioning, or there is a kinetic mass transfer rate between phases. For each of the three scenarios, the concentration in both phases is set to be zero at the top and bottom of the column. At the top this boundary condition is physically reasonable as the top of the column is connected to an infinite clean reservoir of air. For the simulations presented, the contaminant does not reach the bottom boundary, and so the boundary effects are minimal. The contaminant has an initial concentration of $c_w = 1.0$ at depths 30-35 cm. The initial concentration in the water phase at all other depths is zero. The initial air concentration is assumed to be zero. For the purposes of this work, normalized concentrations have been used so that the concentration ranges from 0.0 to 1.0. The results can be rescaled to more realistic values if desired. These boundary and initial conditions correspond to a situation where there has been a contaminant release below the soil surface, such as at a buried waste disposal site. The transport equation is solved to trace the contaminants path under an infiltration event. The transport parameters for the model are taken from the paper by Cho and Jaffe (1990). The dispersivity in both

Figure 3-1 Flow of air and water in a 100 cm column with a water flux of 20cm/h at the surface. Water content at a given time in the column is shown in gray scale by a vertical slice through the diagram. Air particle paths are delineated by the lines on the diagram.

3-4. Kinetic mass transfer in one dimension

phases is set to be $\alpha_w = \alpha_a = 0.3 \text{ cm}$. The molecular diffusion constant in the air phase for TCE was found by Cho and Jaffe (1990) to be $D_{ma} = 0.0756 \text{ cm}^2 \text{ s}^{-1}$, and in the water phase it was $D_{mw} = 1 \times 10^{-5} \text{ cm}^2 \text{ s}^{-1}$.

3-4-1. Transport in water phase only

The first case is where the contaminant does not partition into the air phase. This can be modelled using the equilibrium transport equations with Henry's constant H set to be zero. Under these conditions the contaminant plume evolves as shown in Figure 3-2. The contaminant does not move until the infiltrating water reaches it. Once the infiltrating water reaches the contaminant it moves with the velocity of the water and disperses with time.

3-4-2. Equilibrium partitioning

Equilibrium partitioning for TCE can be modelled by setting Henry's constant $H = 0.392$ (Cho and Jaffe 1990). With this value of Henry's constant, the equilibrium model predicts a concentration profile shown in Figure 3-3. From the figure it can be seen that the contaminant concentration in the water phase instantly equilibrates with the concentration in the air phase. The contaminant then diffuses more quickly in the air phase than in the water phase, resulting in greater spreading than was observed when the contaminant moves only in the water phase. The center of mass of the contaminant plume does not move very much from the original position. This is because for the equilibrium case the velocity of the centre of mass of the contaminant plume is given by:

$$v = \frac{(q_w + Hq_a)}{(R\theta_w + H\theta_a)}$$

As the flux of the air and water phases have opposite signs, the net advection of the contaminant is small.

3-4-3. Kinetic mass transfer

A kinetic mass transfer process greatly affects the spread and path of the pollutant. The kinetic mass transfer model used in this study is the one proposed by Cho and Jaffe (1990) to model TCE movement in a one-dimensional laboratory column study. They fitted their model to experimental data. The values of kinetic mass transfer coefficient obtained ranged in value from 0.03 h^{-1} to 38.08 h^{-1} . This wide range of values reflected different values of dispersion predicted by their model and also took into account the effect of immobile water on the transport process. For the simulation presented here a value of

$K = 0.07 \text{ h}^{-1}$ was chosen to be at the lower end of the range of values observed by Cho and Jaffe to illustrate the potential of the kinetic mass transfer coefficient to alter the observed contaminant distribution. The observed contaminant distribution is illustrated in Figure 3-4 for the water phase and Figure 3-5 for the air phase. The contaminant is initially all in the water phase. Unlike in the equilibrium partitioning case, the contaminant concentration in the air phase builds up slowly, while the water phase concentration can be seen to be decreasing in time in the first 30 minutes. Then the infiltrating water from the surface reaches the contaminant and it is advected downwards as it was in the case where the contaminant was only carried in the water phase. The enhanced diffusion seen in the equilibrium case is also not apparent here as the contaminant takes too long to partition back into the water phase from the air phase. In the air phase, concentrations are much lower than in the equilibrium case where the concentration was $c_a = Hc_w$. The air phase contaminant also carries all the way to the ground surface and is vented to the atmosphere. This can be observed in the figure where there are steep gradients of air concentration at the surface.

With the chosen boundary conditions there is no advective flux across the surface ($qc=0$), but the diffusive flux $D \frac{\partial c}{\partial z}$ is large.

Venting to the atmosphere of contaminant is not predicted with an equilibrium model as the contaminant equilibrates with the clean water that is flowing down from the surface.

These observations have implications for waste disposal site evaluation and design. If it is desirable to prevent the escape of contaminants through the soil surface in the air phase it may be important to include kinetic mass transfer effects in the model. As can be seen from the results above, the type of partitioning chosen between the air and water phases can greatly influence the predicted contaminant distribution in the soil.

Figure 3-2 *Contaminant transport only in the water phase. Concentration profiles with depth are shown at 10 minute intervals.*

Figure 3-3 TCE contaminant plume evolution in time with equilibrium partitioning between the water and air phases.

Figure 3-4 *Concentration in the water phase with a kinetic mass transfer between the water and air phases.*

Figure 3-5 Air concentration for kinetic mass transfer of pollutants with $c_w=1$ initially in the water phase at 30-35 cm depth.

3-5. Two-dimensional contaminant transport

The finite element method with a fine spatial and temporal discretization is able to adequately solve the transport equation in one dimension. In this section the transport equation in two dimensions is solved. The methodology is a direct extension of the one-dimensional case. However, there are some additional complications arising in higher dimensions that must be addressed.

The two-dimensional finite elements will be developed for the case of equilibrium partitioning. As was seen above, the extension of the method to include the kinetic mass transfer process is straightforward when using the finite element method. The governing equation for the equilibrium partitioning case was given in (Eq. 3-2):

$$L(c) = \frac{\partial(\theta c)}{\partial t} + \nabla \cdot (qc) - \nabla \cdot (D \cdot \nabla c) + \lambda c = F$$

The equation is discretized in time using an Euler backward scheme. This scheme is the most stable of the temporal discretizations considered in one dimension and the most effective in controlling oscillations. The two-dimensional finite element scheme is highly prone to oscillations and the most effective scheme for controlling these must be chosen. The finite element procedure is then developed from the weak form of the equation:

$$\int_{\Omega} (L(c) - F) \phi_i d\Omega = 0$$

After application of the Euler backward difference scheme to (Eq. 3-2) and the application of Green's theorem to the spatial derivatives, the equation can be written:

$$\begin{aligned} & \int_{\Omega} \frac{(\theta c)^{n+1}}{\Delta t} \phi_i d\Omega - \int_{\Omega} (qc)^{n+1} \cdot \nabla \phi_i d\Omega + \int_{\Omega} (D^{n+1} \nabla c^{n+1}) \cdot \nabla \phi_i d\Omega \\ & + \int_{\Omega} \lambda c^{n+1} \phi_i d\Omega \\ & = \int_{\Omega} \frac{(\theta c)^n}{\Delta t} \phi_i d\Omega + \int_{\Omega} F^{n+1} \phi_i d\Omega + \int_{\partial\Omega} \{ (qc - D \nabla c)^{n+1} \cdot n |_{\partial\Omega} \} \phi_i dS \end{aligned} \quad (\text{Eq. 3-9})$$

The domain is discretized into rectangles of size $\Delta x_i = x_{i+1} - x_i$ in the horizontal direction and

$\Delta z_i = z_{i+1} - z_i$ in the vertical dimension. The basis and trial functions are chosen to be the piecewise bilinear functions defined on the rectangular elements. The resulting elemental matrices are direct extensions of those in one dimension, see Section 3-3. Binning (1994) provides detailed elemental integrals and matrices for the two-dimensional case.

3-5-1. Lumping in space by numerical integration

Lumping is frequently used to control oscillatory behavior. In one dimension, it was shown in Binning (1994) that temporal lumping does not improve the finite element solution. However, in two dimensions, oscillations in finite element solutions tend to be more pronounced than their one-dimensional counterparts. This is because standard two-dimensional finite element approximations involve nine unknowns per equation, while analogous finite difference approximations often involve only five unknowns. The nine-point approximation can lead to oscillatory solutions even in the absence of advection. For example, con-

sider the simple two-dimensional diffusion equation, $\frac{\partial c}{\partial t} = D \nabla^2 c$ defined on the domain illustrated in Figure 3-6. If there are no flow boundaries on all sides and a fixed concentration of $c=1$ at node 2, the consistent finite element solution will con-

Figure 3-6 Domain for model problem $\frac{\partial c}{\partial t} = D \nabla^2 c$.

tain oscillations for $\rho = \frac{D \Delta t}{\Delta x^2} < \frac{1}{3}$. For $\rho > \frac{1}{3}$ the solution will not contain oscillations. In contrast with the consistent finite

element scheme, a five point finite difference solution is nonoscillatory for all ρ . The consistent finite element discretizes the dispersion using a nine spot approximation which gives undue emphasis to diagonal coupling across the element. A lumping scheme must be chosen to decouple the diagonals of the element. Zienkiewicz (1989) suggests several lumping schemes. The lumping scheme used here is to replace the exact integrals evaluated above with a 4 point integration rule with the integration points chosen to be at the four corners of the element. That is:

$$\int_{\Omega_e} F(x, z) d\Omega = \frac{|\Omega_e|}{4} \sum_{i=1}^4 F(x_i, z_i)$$

Using the lumped matrices a finite element approximation is derived that closely resembles a five point centered-in-space finite difference scheme. The only term which contains information across the diagonal of an element is the off-diagonal terms in the dispersion tensor. Use of this finite element scheme results in an approximation of the dispersion that is non-oscillatory. This was confirmed by simple numerical studies of the model equation. Note that oscillations may still arise in the solution of the full transport equations because of the presence of the advective term. To control this type of phase-shift oscillations, sufficiently fine spatial and temporal resolution is used in the example problems discussed herein.

3-5-2. Mass balance

The mass balance of the finite element method is very good. The transport equation solved is a linear equation and is in conservative form. If the finite element equations are summed over the domain, the advection and dispersion terms cancel on the interior element boundaries. A mass balance ratio is defined as the total change of mass in the domain divided by the mass influx from sources and sinks and through the boundary:

$$\frac{\sum_{i=1}^N ((\theta c)_i^{n+1} - (\theta c)_i^n) \int_{\Omega} \phi_i d\Omega}{\sum_{i=1}^N \int_{\Omega} F^{n+1} \phi_i d\Omega + \int_{\partial\Omega} \{ (qc - D \nabla c)^{n+1} \cdot \mathbf{n} \}_{\partial\Omega} \phi_i dS} = 1$$

The mass balance ratio for the finite element method was calculated in the program and was found to be very close to one.

3-5-3. Example simulations

A number of verification simulations, with accompanying analyses, have been reported by Binning (1994). For example, consider a case of a strip-source of contamination along the top boundary of a two-dimensional domain, in a constant-moisture-content flow field. This corresponds to the relatively simple case of saturated flow and associated contaminant transport, for which an analytical solutions may be found. The domain considered is of size 3.0 x 6.0cm. The moisture content in the domain is fixed at 0.37 and the flux is in the z direction with magnitude 0.37cm/s. This flux and moisture content lead to an average fluid velocity of 1.0 cm/s. The dispersivity is 0.01cm. The concentration is initially set to be $c=0.0\text{g/cm}^3$ and there is a strip source of contaminant of length 1.0cm and strength $c=1.0\text{g/cm}^3$ on the top of the domain at one side. While these dimensions used in this demonstration problem are small, they will demonstrate the properties of the method. An analytical solution to this problem was found by Domineco and Robbins (1985) and is illustrated in Figure 3-7. The lumped finite element solution for a relatively fine grid of $\Delta x = \Delta z = 0.1\text{cm}$ is shown in Figure 3-8. The Peclet number in Figure 3-8 it is 10. The time step is chosen to have size 0.1s, corresponding to a Courant number of 1.0. This value of Peclet and Courant is within the bounds given in Section 3-3-1. for acceptable solutions. An error measure giving the average absolute error at each node can be defined as:

$$\text{error} = \frac{1}{N} \sum_{i=1}^N |c_i^{\text{numerical}} - c^{\text{analytical}}(x_i, z_i)|$$

The error for the finite element scheme found using this error measure is 0.009.

To examine the transport solution under transient moisture contents in the unsaturated zone, consider the example flow problem of Section 2-5. Assume now that the infiltrating water carries with it a dissolved contaminant with normalized concentration $c=1$. The finite element solution for this case is shown in Figure 3-9, assuming no partitioning into the air phase. The results demonstrate that the contaminant front moves into the subsurface at a slightly slower rate than the moisture front, as is expected in unsaturated systems. For this simulation, the concentration mass balance is essentially 100 percent.

Other examples, including transport associated with transient flow in heterogeneous systems, may be found in Binning (1994).

3-6. Gas phase migration from designed LLW containment facilities

3-6-1. Design of LLW disposal facilities

Historically, the design of low-level radioactive waste (LLW) disposal facilities has focused on controlling infiltrating water. In this way, transport to the saturated groundwater zone is limited, if not prevented. Gas-phase migration of volatile compounds is often neglected in the facility design, although such migration may represent a significant exposure pathway (see, for example, Kunz 1982, Metcalfe and Farquhar 1987). As an example of the possible importance of air-phase contaminant transport, a model facility design is analyzed. The model design is based on design specifications provided by the U. S. Nuclear Regulatory Commission staff (personal communication, NRC 1993).

The hypothetical facility design involves 60 buried concrete vaults capable of storing a total of approximately 7×10^6 cubic feet of Class A low-level waste. Each vault covers an area of approximately 170,000 ft², and is made up of 24 containment cells. Each of these cells is overlain by an engineered capillary barrier system composed of layers of different materials, including sand layers and a geomembrane over a three feet thick layer of clay. This capillary barrier is designed to prevent water from infiltrating to the containment structures below. A schematic of the layered system is shown in Figure 3-10.

To prevent buildup of water inside a cell, in the event that water breaches a cell, each cell is designed with a drain system. This consists of a six-inch layer of pea gravel along the floor of each cell, which is sloped toward a four-inch drain pipe. This pipe passes through the wall of the cell, to a larger drain system outside the cell wall (see Figure 3-11). While this design is probably effective in controlling water buildup, it coincidentally provides a direct conduit for extra-cell migration of gas-phase contaminants. Therefore, if any gas-producing processes occur within the cell, such as carbon-14 based methane production from biologic activity, then the drain system will act as a source of gas-phase contaminants to the surrounding porous medium.

3-6-2. Biologic methane production

In a facility designed to accept low level radioactive waste it is expected that some of the waste would contain the radioactive species carbon -14 which has a half life of 5730 years. The radioactive carbon present in the waste would act as an

Figure 3-7 Analytical solution for contaminant transport from a strip source of length 1 cm at the top left of the domain. The dispersivities were set to be $\alpha_L = \alpha_T = 0.01$ cm and the fluid velocity was constant at 1 cm/s in the z direction, with a constant moisture content of 0.37. The solution is shown at $t=3.0$ s.

Figure 3-8 *Lumped finite element solution of the problem illustrated in Figure 3-7 on a grid with $\Delta x = \Delta z = 0.1\text{cm}$.*

Figure 3-9 Contaminant transport solution for infiltration into a homogeneous material using the velocities of water obtained from the solution shown in Figure 2-11.

Figure 3-10 *Multilayered capillary barrier system over the containment cells.*

Figure 3-11 Subsurface concrete cell drainage system.

energy source for microbes. By-products of microbial digestion of the carbon source would include carbon dioxide and methane. The production of methane containing carbon-14 has been observed at an operational low-level radioactive waste disposal site near West Valley, New York (Kunz 1982).

In any landfill it is expected that microbes will degrade various carbon sources to methane, carbon dioxide and biomass. The production of these products is dependant on the environment surrounding the organisms. Prediction of the environment within a containment cell appears to be highly uncertain, and is beyond the scope of this report. However, it seems very likely that the environment within the cells will be depleted of oxygen, such that some carbon-based materials will degrade anaerobically. For example, a typical stoichiometric relation for anaerobic biodegradation of cellulose (a major component of wood products such as paper and packaging materials) can be represented as follows (EMCON Associates 1980):

where $C_6H_{10}O_5$ represents a stoichiometric equation for cellulose. As a simple model, it might be assumed that microbes will produce methane at a relatively steady rate once the environment becomes stable. This leads to a contaminant source term for the air phase. The water in the reaction can be derived from the natural moisture content of the waste materials.

3-6-3. Application of the two-phase air and water flow and contaminant transport model to the facility design

Using the simulation code described above, the designed facility may be modeled to gain insight into possible pathways for vapor-phase contaminant migration. Once gases escape the containment cell (presumably via the drain system), there are two possible pathways to the land surface. The first is diffusion of the contaminant through the capillary barrier system; the second is migration around the layered system to the perimeter of the vault. These pathways are considered below. Migration to the water table, and subsequent dissolution into and movement with the groundwater, is not considered herein but may be important for some contaminants.

3-6-4. Vapor phase diffusion through the layered system

To estimate possible mass flux through the capillary barrier system, several assumptions are made. First, because no material properties are presented for the "sand" and "clay" used in the design, tabulated values of van Genuchten parameters, based on generic "sand" and "clay" materials, have been used to characterize the necessary unsaturated hydraulic properties. Because of lack of information, and the desire to provide a conservative estimate, the geomembrane was eliminated from consideration. The layered system used in the simulations is shown in Figure 3-12. The van Genuchten unsaturated flow parameters assigned to the different materials are given in Table 3-3.

A critical consideration in the diffusive flux calculation is the choice of expressions for air-phase diffusion coefficients, and the assignment (or determination) of moisture contents. As discussed in Section 1.5.1, the expression of Fluhler (1973) was chosen, so that

$$D_{m_a}^{eff} = D_{m_a} \theta_a \tau_o \left(\frac{\theta_a}{\phi} \right)^{3.25} \quad (\text{Eq. 3-10})$$

where $\tau_o = 0.66$, D_{m_a} is the free air molecular diffusion coefficient, and θ_a is the air content (volume of air / total volume). See Section 1.5.1, and associated Figure 1-2, for a discussion of the different formulations for air-phase diffusion coefficients.

To demonstrate the importance of the diffusion coefficient, a simple comparison was made using the formulations for air-phase diffusion presented by Lai et al. (1976) and Fluhler (1973). A constant diffusion coefficient was also used for comparison (see Figure 1-2). For a one-dimensional layered system such as that shown in Figure 3-12, with clay assumed to be at a water saturation of 90% ($S_a = 0.1$) and with concentration fixed at constant values of 1 at the bottom and 0 at the top, the steady-state flux through the system differs by more than two orders of magnitude. In addition, the time to steady state varies

Figure 3-12 Layered system used in the one - dimensional simulations.

from hours (constant diffusion coefficient) to tens of years (formulation of Fluhler). Table 3-2 and Figure 1-2 demonstrate these results.

Table 3-2 *Summary of formulation differences for the effective molecular diffusion coefficient.*

Formulation	Constant $D^{eff} = 0.24$	Lai et al (1976)	Fluhler (1973)
Time to Steady State	hours	2 weeks	20 years
Diffusive flux at Steady State (mass/cm ² s)	360×10^{-6}	70×10^{-6}	1×10^{-6}

3-6-5. Vapor-phase migration to the perimeter of the vault

To examine contaminant migration to the edge of the covered areas, and subsequently to the land surface, a two-dimensional cross-sectional model of the containment cell system was developed. Figure 3-13 illustrates the cross-section to be modeled. The materials of interest in this model are the clay, layers of sand above the clay, backfill sand, and native soil. For this model the layered system is simplified to include only two layers, the clay and the over layer of sandy material. The source of contamination is assumed to be methane gas production from microbial activity within the containment cell. The drain pipe engineered into the system serves as the direct conduit to the porous media surrounding the cells.

The numerical methods used to solve the two-dimensional equations are described in Section 3-5. The numerical grid and associated boundary conditions are illustrated in Figure 3-14. Unsaturated flow parameters used in the model are given in Table 3-3.

Table 3-3 *Van Genuchten parameters in layered system model.*

Layer	Model	Porosity	θ_s	θ_r	α	n	k_{ws} (cm/s)	k_{as} (cm/s)
Clay	1D, 2D	0.42	0.37	0.06	0.029	1.1	4.0×10^{-8}	7.2×10^{-6}
Silty Sand	1D	0.37	0.31	0.05	0.04	1.5	5.0×10^{-4}	0.09
Sand	1D, 2D	0.36	0.31	0.12	0.06	1.38	0.0042	0.77
Native Material Case 1	2D	0.36	0.31	0.12	0.06	1.38	0.0042	0.77
Native Material Case 2, 3	2D	0.37	0.35	0.12	0.10	2.2	1.6×10^{-4}	0.03

3-6-6. Source term

Biologic activity in the reinforced concrete cells is expected to produce radioactive gases including carbon dioxide and methane. Gas production should reach a steady rate when the microbe population stabilizes. This rate of production will be the source term for the two dimensional model.

Data from the LLW disposal facility in West Valley New York indicated the landfill was producing a maximum of about 7×10^{-3} cubic centimeters of radioactive gas per second for each cubic meter of waste (Kunz 1982). At the West Valley site waste was buried in shallow trenches with minimal protection against infiltration. The moist environment of the waste at the West Valley site would act to enhance methane and carbon dioxide production.

The infiltration controls of the designed landfill would be expected to reduce significantly the amount of moisture available in the subsurface for biologic activity, thereby reducing the production of radioactive gases. Because the actual rate of gas production in a containment cell is unknown, a fraction of the West Valley production rate is taken to serve as an illustrative example. In this work a value of 1% of the West Valley rate is used as the source term. Lack of information about the

Figure 3-13 Cross-section of vault layers to be modeled in two dimensions.

Figure 3-14 Discretization and boundary conditions for two-dimensional simulation.

3-6. Gas phase migration from designed LLW containment facilities

expected environmental conditions within a containment cell, and the concomitant lack of information about gas production rates, are a major source of uncertainty in this model.

3-6-7. Assumptions

To model this two-dimensional slice of the vault, several assumptions are made. The first assumption made is that the moisture content in the porous media surrounding the containment cells is at steady state. The sandy materials below the clay layer are assumed to have relatively low moisture contents, while the clay maintains a relatively high moisture content. While some short-term fluctuations in moisture content might be expected, the approximation of long-term steady-state behavior seems reasonable.

The geomembrane present in the LLW design is not included here. Our results will show that even without the geomembrane the amount of contaminant flux through the containment layers is negligible.

The air phase is assumed to have reached some steady state of flux. This model assumes that the microbes which produce methane have reached their stationary state and are producing methane at a constant rate. The rate used in the model is chosen to be 1% of the observed value for a similar volume of waste found at the West Valley NY LLW disposal site. Water is an essential component in anaerobic degradation. The West Valley site has no provisions to keep water out of the system and so biodegradation is expected to occur there at a faster rate than at the modelled site which is designed to keep water out.

The boundary conditions of the model are shown in Figure 3-14. The left side of the system is assumed to be a no flow boundary to water and air and zero flux across the boundary for concentration. This boundary condition is reasonable given the symmetry of the overall design of the waste site. The top of the model represents the atmosphere above the site. The concentration of methane in ambient air is assumed to be zero; a constant air pressure of zero is also assigned to this boundary. The bottom of the model is assigned as a no flow boundary to water and air and is a zero flux boundary for concentration. The top portion of the right side boundary is assigned to be no flow for water, air and a zero flux boundary for concentration. The bottom element along the right boundary is assigned a constant flux to air, zero flux water, and a concentration of unity. Thus this bottom corner represents the outflow of the drainage pipe from the reinforced concrete cells.

3-6-8. Results of the model

Three cases of the two dimensional model were simulated. In the first two cases the source term is 1% of the West Valley production rates, which induces advection in the system. In the third case the mean velocity of the air as well as the water is assumed to be zero, with the same concentration boundary conditions as the other runs. This case corresponds to assuming that methane production is taking place but at a rate such that the dominant transport mechanism is molecular diffusion in the air phase. Material properties relevant to the two dimensional model runs are given in Table 3-3.

This proposed design for LLW disposal is a general design, it is not intended to be specific for any particular site. For this reason the type of soil to be encountered as native to the construction site is an unknown in the system. The first two cases explore the effects of a change in unsaturated flow properties of the native soil on the system. In Case 1 the native material is a sand. Figure 3-15 shows the moisture content and air-phase particle flow vectors three months into the simulation for Case 1. Figure 3-16a through Figure 3-16c demonstrate the resulting concentration profiles at a series of times. The contaminant requires approximately 3 years to break through at the perimeter of the site.

Today it is considered unlikely that a LLW disposal site would be chosen to be constructed on a sand (Case 1). Case 2 uses a more realistic native material a sandy loam. The moisture content and air particle flow vectors for Case 2 are shown in Figure 3-17 and the resulting series of concentration profiles are depicted in Figure 3-16a through Figure 3-16c. When comparing Figure 3-15 and Figure 3-17 significant differences in the path taken by air particles are apparent with the air preferentially flowing through the higher conductivity sand material. However, the contaminant transport solutions are similar for the two cases, with breakthrough occurring at 3 years.

Actual rates of methane production could be much lower than those modelled above. The limiting case, explored here as Case 3, assumes that no advection takes place in the system and transport of the contaminant out of the vault is by diffusion only. The resulting concentration profiles for a series of times is shown in Figure 3-16a through Figure 3-16c. In this case breakthrough occurs in 20 years and the profile shown at 100 years time, Figure 3-16c, is essentially a steady state condition. This case represents an upper bound on the expected breakthrough time for contaminants to reach the surface. In practice cases one and two demonstrate that the breakthrough may occur in significantly shorter times than those predicted by assuming that the main transport mechanism is through diffusion.

Figure 3-15 Case 1 moisture content contours and air particle movement vectors at 3 months.

3-6. Gas phase migration from designed LLW containment facilities

Figure 3-16 Case 1 concentration profiles; (a) time = 3 months, (b) time = 3 years, (c) time = 8 years.

Figure 3-17 *Case 2 moisture content contours and air particle movement vectors at 3 months.*

Figure 3-18 Case 2 concentration profiles; (a) time = 3 months, (b) time = 3 years, (c) time = 8 years.

Figure 3-19 Case 3 concentration profiles; (a) time = 5 years, (b) time = 20 years, (c) time = 100 years.

3-7. Discussion

The transport simulators described in this section use standard finite element methods with special reduced integration routines to produce lumping of the approximations which are shown to give better solutions than consistent approximations. As with the two-pressure formulation for the flow equations, this numerical method is robust, easy to program, and has numerical behavior that is well-known. In particular, the method requires relatively fine discretization governed by restrictions on the grid Peclet and Courant numbers. Within these constraints, the numerical method behaves very well. Similar restrictions on numerical discretization also apply to the solution of the multiphase flow equations. In fact, a mesh that is sufficiently fine to provide a solution to the multiphase flow equations will also provide a good solution to the transport equation.

Other numerical techniques can be used to solve the transport problem more efficiently, for example the Eulerian Lagrangian Localized Adjoint Method of Binning (1994). This method takes advantage of the characteristics of the governing equation and does not have a restriction on the Courant number as is found in the finite element method. However this method is not used here as the finite element method is simple and robust and when coupled to the solution of the multiphase flow equations, the majority of the computational effort lies in the solution of the nonlinear flow equations. Any improvements in the solution of the transport equation are unlikely to significantly alter the computational effort in solving the combined flow and transport problem.

The simulator described in this section may be used to illustrate several important general principles regarding contaminant transport in unsaturated soils. First, when considering problems in the short-time range, the partitioning behavior of the contaminant may be significant when considering contaminant fluxes at the land surface. In particular, for kinetic partitioning described with the formulation proposed by Cho and Jaffe (1990), the time scale associated with partitioning from the air phase to the water phase is longer than that associated with the flow dynamics. Therefore contaminant can out-gas from the soil to the atmosphere. For equilibrium partitioning, such out-gassing does not occur in the example considered. Rather, apparently-enhanced mixing occurs because of the different velocities associated with the water and air phases. In short-time cases with kinetic partitioning, the general result is that with different directions of flow of the water and air phases, the phase within which the contaminant resides must be identified. The exchange characteristics between phases must also be known. With this information, reasonable estimates of contaminant movement can be made.

For long-time transport problems, kinetic partitioning is not likely to be important. In addition, long-term moisture content may be essentially constant, depending on the system under consideration. The moisture content of the system will have a significant influence on the air-phase diffusion coefficient, which in turn may have a significant effect on the overall contaminant transport. For the engineered system considered for low-level radioactive waste disposal, moisture content is likely to be essentially constant over major parts of the domain. Two key components of the transport analysis for this system are the actual moisture content values (thereby determining the effective diffusion coefficient) and the source term for the contaminant. In these long-term analyses, the resulting flow system tends to be significantly simpler than those in the short-term problems.

One especially interesting observation about the specific LLW site design discussed above is that the design has a simple air-phase transport pathway built into it. The drainage system, designed to drain water out of each containment cell, will allow a direct pathway for air-phase contaminants to migrate from within the containment cell to the surrounding unsaturated porous medium. The contaminants then move by advection and/or diffusion/dispersion through the unsaturated zone, eventually reaching the land surface. While uncertainties about the source term make it difficult to determine whether or not this is a significant transport pathway, the engineering design of the facility might be reconsidered in light of the existence of this direct air-phase pathway.

3-8. References

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Closing Remarks

This document describes a general model of fluid flow and contaminant transport in unsaturated soils. The unsaturated zone is viewed as a two-fluid-phase system, and the dynamic behavior of both the water and air phases is included in the model. Contaminant transport is considered in both the air and water phases, with both equilibrium and kinetic partitioning between the fluid phases. Solid-phase interactions are also included via a retardation coefficient.

The model was applied to a number of scenarios in both one and two dimensions. The examples were chosen to demonstrate certain general behaviors that pertain to unsaturated soil systems. The first of these is the simple but important observation that the air phase is dynamic; the often-stated assumption that the air phase is stagnant is incorrect, leading to a qualitative picture of the unsaturated zone that is at best misleading. For short-term analyses, the dynamic response of the air phase may be quite important in the context of contaminant transport. This is true independent of the validity of Richards' equation to describe the water-phase movement.

A second observation involves time scales. For short-term problems, full system dynamics will usually be important. In addition, kinetic partitioning of the contaminant between the water and air phases can be quite important. Conversely, for long-term problems, the system might be simplified from the fully dynamic description such that, for example, kinetic partitioning may be neglected. Over long time scales, certain short-term effects may be manifested as apparent increases in mixing coefficients (an effect analogous to that shown in Figure 3-3 for equilibrium partitioning).

The general model described in this document covers both short-term and long-term situations. As such, it provides a useful tool to help in the analysis of complex unsaturated-zone transport problems such as those associated with LLW disposal sites. However, because of the difficulties associated with analysis of these extremely complex systems, this and any other model should be applied with caution.

More than most other waste-disposal problems, low-level radioactive waste disposal is extra-ordinarily difficult to analyze because of the long times involved. Low-level waste disposal sites must be designed to immobilize and contain hazardous materials for hundreds to thousands of years. The successful design of such long-term structures requires prediction of their performance beyond the time scales for which we have knowledge of the behavior of materials and designs in current use. Assumptions about the behavior of constructed facilities, the behavior of natural materials, the nature of forcing functions and source terms, and many other aspects of the problem mean that the numerical model should be viewed as a tool to provide engineering insights as opposed to one which provides a detailed and definitive prediction.

This philosophy is consistent with the discussions presented by Konikow and Bredehoeft (1992), wherein the ability of groundwater models to provide meaningful predictions was studied. In that work, saturated groundwater flow systems were considered; these are much simpler than unsaturated systems. In addition, the time scale of future predictions was usually on the order of years to perhaps a decade; this is much shorter than the time scales involved in LLW problems. Perhaps the most interesting findings in the work of Konikow and Bredehoeft (1992) were related to post-audits of previous modeling studies. These post-audits indicated that the predictive ability of models generally has an upper limit corresponding to a time scale of the order of the length of history-matching used to calibrate the model. This reinforces the view that the model must be viewed as one of a suite of analysis tools that can be used to make a "best engineering" judgement.

The two-phase unsaturated zone model described herein is a general numerical analysis tool for developing such an engineering judgement. The model should be used to aid the decision maker in developing an intuition for the physical processes that are important in the design of a waste repository.

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Appendix

Two-Phase (air and water) One-Dimensional Flow and Transport Code

written by Philip Binning,

based on the work of M.A. Celia and Philip Binning
A Mass Conservative Numerical Solution for Two-Phase flow in Porous
Media With Application to Unsaturated Flow, *Water Resources
Research*, Vol. 28, No. 10, Pages 2819-2828, 1992.

Appendix: Contents

1. Introduction	1
2. Flow Equation Formulation	1
3. Transport Equation Formulation	1
Governing Equations	1
Vapor-liquid equilibria.	1
Equilibrium Mass Transfer	2
Non-Equilibrium Partitioning	2
Sorption	3
Numerical Method	3
4. Units and Other Conventions.	3
5. Input Files	3
Format of input file	3
6. Sample Input File	4
7. Input variables	4
Space discretization	4
Time stepping	4
Variable Time stepping	5
Convergence criteria	5
Initial Conditions	5
Flow Boundary Conditions	6
Angle of column	6
Fluid Properties	6
Ponding	6
Soil Properties	7
Transport parameters	7
Printing Control	8
8. Example Input Files included with code	9
83open.in	9
83closed.in	9
20open.in	9
20closed.in	9
wonly.in	9
eq.in	9
noneq.in	9
9. Output Files	9
10. Sample Output	10
11. Graphics Output	18
p.x	18
theta.x	19
qw.x	20
qa.x	21
infiltr.x	22
massbal.x	23
dt.x	24
iter.x	25
cw.x	26
ca.x	27
12. Errors	28
Input File	28

Memory	28
13. References	28
14. Program Structure	29
15. Compilation	29
Compiling on the IBM PC	29
Compiling with a UNIX machine	29

1. Introduction

The One-Dimensional Two Phase code was developed to study the flow air and water and the transport of contaminants in the unsaturated zone. The code was originally developed as a research tool but has been extensively revised and improved to allow its use as an educational tool for understanding multiphase flow in the unsaturated zone.

The code has the following features:

- * Complete solution of both the air and water flow equations. The code outputs; the pressures and flux of both phases, the moisture content, cumulative infiltration, time step size, and mass balance error.
- * Complete solution of the contaminant transport equations in both phases including reactions and equilibrium/kinetic mass transfer between phases.
- * User definable soil properties. The code currently supports Parker's (1989) generalization of Van Genuchten's (1980) functional forms. Modification of the code to incorporate other functional forms is not difficult.
- * Variable sized time stepping with user control of output times.
- * Time varying boundary conditions
- * Hydrostatic and constant initial conditions
- * Variable angle of column (Any angle from horizontal to vertical can be considered)

2. Flow equation formulation

The details of the governing flow equations can be found in the reference that is printed on the cover.

3. Transport equation formulation

Governing equations

For each phase, the equations for the transport of contaminants can be written:

$$\frac{\partial(\theta_{\alpha} c_{\alpha})}{\partial t} + \frac{\partial}{\partial z}(q_{\alpha} c_{\alpha}) - \frac{\partial}{\partial z}\left(\theta_{\alpha} D_{\alpha} \frac{\partial c_{\alpha}}{\partial z}\right) + \lambda_{\alpha} \theta_{\alpha} c_{\alpha} = F^{\alpha} \quad \alpha = \text{air, water}$$

where:

- θ_{α} phase content of phase α []
- c_{α} concentration of phase α [M]/[L³]
- q_{α} flux of phase α [L]/[T]
- D_{α} Dispersion of phase α [L²]/[T], $D_{\alpha} = \alpha q_{\alpha} + \theta_{\alpha} D_m$
- α dispersivity coefficient [L]
- D_m molecular diffusion coefficient [L²]/[T]
- λ_{α} Chemical/radioactive decay rate 1/[T]
- F^{α} Source/Sink term

The first term describes the change of mass with time, the second the advective flux, the third the diffusive flux and the fourth the decay of pollutants through chemical or radioactive reactions. The right hand side describes source/sinks of contaminant mass.

Vapor-liquid equilibria.

Modeling the simultaneous transport of two phases requires a description of the mass transfer processes between the individual phases. The program has two options, either the concentration in each phase is assumed to be at equilibrium or the phase exchange of mass follows a kinetic mass transfer law.

Equilibrium mass transfer

Under the equilibrium assumption, mass is assumed to exchange instantaneously between phases. The concentration in each phase is proportional to the concentration in the other phase. They are related by Henry's Law:

$$\frac{c_a}{c_w} = H$$

where H is called the Henry's constant. Henry's law is usually written in terms of the partial pressure of the contaminant in the vapor phase $P_c = K_H x_c$, where P_c is the partial pressure of the contaminant in the air phase, K_H is the Henry's law constant $[T^2]/[L][M]$, and x_c is the mole fraction of the contaminant in the water phase. By applying the ideal gas law and the definition of a mole fraction, H can be seen to be related to K_H by the following:

$$H = K_H \frac{MW_c MW_{H_2O}}{\rho_{H_2O} MW_c RT}$$

where MW is the molecular weight of either the contaminant or water, ρ is the density of water, R is the real gas constant, and T the temperature in $^{\circ}K$. Under the equilibrium assumption the air concentration is directly proportional to the water concentration so the individual phase mass balance equations can be added to give one equation in water concentration:

$$\frac{\partial((\theta_w + H\theta_a)c_w)}{\partial t} + \frac{\partial}{\partial z}((q_w + Hq_a)c_w) - \frac{\partial}{\partial z}((\theta_w D_w + \theta_a H D_a) \frac{\partial c_w}{\partial z}) + (\lambda_w \theta_w + H\lambda_a \theta_a)c_w = 0$$

Non-equilibrium partitioning

Cho and Jaffe (1990) conducted laboratory experiments that suggested that an equilibrium assumption may not be valid in a dynamic system and developed a kinetic phase transfer model. Their experiments suggested that the contaminant moved from one phase to the other at a rate determined by the degree of disequilibrium, a kinetic phase transfer coefficient and the water content. For the transfer between phases they wrote the equations:

$$\frac{dc_w}{dt} = K\theta_a(c_a - Hc_w)$$

$$\frac{dc_a}{dt} = -K\theta_a(c_a - Hc_w)$$

where K is the coefficient of mass transfer $[L]/[T]$. The mass transfer coefficient reflects the ease with which mass can move between the phases and will depend on the contaminant and porous medium properties. In the transport equation, the mass transfer equations appear as source and sink terms in the right hand side. When using kinetic mass transfer the transport equations for both phases must be used.

$$\frac{\partial(\theta_w c_w)}{\partial t} + \frac{\partial}{\partial z}(q_w c_w) - \frac{\partial}{\partial z}(\theta_w D_w \frac{\partial c_w}{\partial z}) + \lambda_w \theta_w c_w = K\theta_a(c_a - Hc_w)$$

$$\frac{\partial(\theta_a c_a)}{\partial t} + \frac{\partial}{\partial z}(q_a c_a) - \frac{\partial}{\partial z}(\theta_a D_a \frac{\partial c_a}{\partial z}) + \lambda_a \theta_a c_a = -K\theta_a(c_a - Hc_w)$$

Sorption

Many pollutants are sorbed onto the solid phase and move at a rate slower than that predicted by the transport equations written above. In the case of sorption the equation for the water phase is modified to include a retardation factor. The principle assumption we will use in deriving a retardation

factor is that the water is the wetting fluid so that the air phase does not have any contact with the solid phase. Thus adsorption can only occur from the water phase into the solid phase. It is assumed that there is a

linear equilibrium Freundlich isotherm between the water phase and the solid phase. The isotherm has the form:

$$\frac{\text{mass of contaminant in solid phase}}{\text{mass solid phase}} = F = k_d c_w$$

where k_d is called the distribution coefficient. The isotherm states that the concentration of contaminant in the solid phase is linearly proportional to that in the water phase. Typical values for this parameter can be found in the text by Domenico and Schwartz (1990). Using this assumption, the equation for the water phase can be modified to include adsorption:

$$\frac{\partial(\theta_w c_w)}{\partial t} + \frac{\partial}{\partial t}(\theta_s \rho_s F) + \frac{\partial}{\partial z}(q_w c_w) - \frac{\partial}{\partial z}(\theta_w D_w \frac{\partial c_w}{\partial z}) + \lambda_w \theta_w c_w = F^w$$

The time derivatives in the above equation can then be rewritten:

$$\frac{\partial(\theta_w c_w)}{\partial t} + \frac{\partial}{\partial t}(\theta_s \rho_s F) = \frac{\partial}{\partial t}(R \theta_w c_w)$$

where R is the retardation coefficient defined by:

$$R = \left(1 + \frac{\theta_s \rho_s k_d}{\theta_w}\right).$$

Numerical method

The transport equations are solved using an Euler backward centered in space finite difference scheme. Full details can be found in Binning (1994).

4. Units and other conventions.

- * The units are assumed to be cgs, that is, centimeters, grams and seconds. (These units are hardwired in the computer code where constants for density and gravity appear).
- * The code assumes that z axis is oriented down with the origin at the surface.
- * The code is set up for air and water.
- * The pressure head is in units of cm of water (i.e. pressure in equivalent water column height $h_a = p_a / \rho_{ow} g$).

5. Input files

There is usually only one input file, 2p.in. However, if the initial conditions are to be read and readic != 0, then the program also reads ic.in. If cinit != 0 then the program also reads cic.in.

Format of input file

The computer code reads each line of the input file separately. As it reads each line it strips all non numeric information out of the line. This means that the user can add their own comments to the input file (Comments should be less than a line long). The user should take care to separate each input parameter by either a tab or space character. Each line of the input file should contain certain parameters. If the user leaves out an input line the rest of the input will be read incorrectly as the program will assume that the correct data should have been there. The format of the input file is described in the next section. If the user has problems creating an input file, they should run the program and check 2p.out. Many errors can be found by careful examination of this file.

6. Sample input file

The following input file is included with the program and is called 83open.in on the distribution disk. It describes a 100cm vertical column, a simulation time of 6000 s using variable time steps, hydro-

static initial condition with a water pressure set at -9.9 cm at the bottom. The water phase is set to have a flux of 0.0023 cm/s (8.3cm/hr) at the surface and a fixed pressure of -9.9 cm at the bottom. The air is set to be at atmospheric pressure at the top and bottom. Ponding is allowed at the surface (but does not occur as the set flux rate is less than the saturated conductivity). The soil is specified to be of Touma and Vauclin (1986) type. In this example the pollutant is a salt tracer and

so transport is allowed only in the water phase. The concentration in the water phase is set to 1 at the top of the column and zero at the bottom. The cover of this manual shows graphics created from this example.

```
nn 26 dz 4.0
dt 10.0 timetot 6000 nprint 6000 maxtime 6000.0
itmin 10 itmax 15 dtdec 0.95 dtinc 1.05
maxiter 40 errorr 1.0e-4 errorh 0.1
readic 0
hydrostaticw 1 hzerow -100.0 hydbotw -9.9
hydrostatica 1 hzeroa 0.0 hydbota 0.1204
timestw 1
fluxtw 1 bctw 0.0023 timetw 6000.0
timesta 1
fluxta 0 bcta 0.0 timeta 6000.0
timesbw 1
fluxbw 0 bcbw -9.9 timebw 6000.0
timesba 1
fluxba 0 bcba 0.1204 timeba 6000.0
dipangle 1.5707
compress 1.0 storativity 2.0e-4
pond 1 hae 14.0
porosity 0.37
type 1
thetar 0.0265 thetas 0.312 alpha 0.044 ng 2.2
kws 0.0042 kas 0.77777777
equilibrium 1 cinit 0
ctimesw 1
cfluxtw 0 ctopw 1.0 ctimew 10000.0
ctimesa 1
cfluxta 0 ctopa 0.0 ctimea 10000.0
cbotw 0.0 cbota 0.0
lambdaw 0.0 lambdab 0.0 rhos 1.0 kd 0.0 k 0.0 h 0.0
alphaa 1.0 alphaw 1.0 dmoleca 0.0756 dmolecw 0.00001
pmatrix 0 reswrite 0 flush 1
vprint 1 nvprint 10
tvprint
600. 1200. 1800. 2400. 3000. 3600. 4200. 4800. 5400. 6000.
```

7. Input variables

Space discretization

```
nn 26 dz 4.0
```

nn number of nodes to be used. Note that the length of the domain = (nn-1)*dz.
dz spacing between nodes.

Time stepping

```
dt 10.0 timetot 6000 nprint 6000 maxtime 6000.0
```

dt time step size.
timetot total amount of time steps. Simulation finishes when this number of steps is exceeded or the time of simulation exceeds maxtime.
nprint Number of time steps between printing information.
maxtime Maximum simulation time in seconds

Variable time stepping

```
itmin 10 itmax 15 dtdec 0.95 dtinc 1.05
```

If variable size time steps are not desired set $dtdec=dtinc=1.0$.

Variable sized time steps can be used to speed up the simulation by allowing the program to use larger time steps when less iterations are needed for the non-linear iteration scheme to converge. The variable size time step option is set by choosing iteration limits that define when the time step can be changed. When the number of iterations exceeds $itmax$ the time step dt is reduced by $dtdec$. When the number of iterations is less than $itmin$, the time step size dt is increased by $dtinc$. As a first try, set $itmin=10$, $itmax=15$, $dtinc=1.05$, $dtdec=0.95$. Other values of these parameters may be required to ensure convergence. If in doubt use fixed time step size.

Note: If using variable sized time steps, use $maxtime$ to define the end of the simulation. Set $nprint$ and $timetot$ to be a large number, and use the option to print output at user defined times (See description of printing control below)

Convergence criteria

$maxiter$ 40 $errorr$ $1.0e-4$ $errorh$ 0.1

$maxiter$	maximum number of iterations allowable. If the nonlinear iteration scheme is unable to converge, this stops the program.
$errorr$	maximum error on the residual. This parameter is dimensionless.
$errorh$	maximum error on the pressure head. (units of pressure head)

These parameters define the accuracy of the desired solution. Generally more accuracy requires more nonlinear iterations and thus more computer time. We have used $errorr=1.0e-4$ and $errorh=0.1$ in most of our work. In the notation of the paper (which is reproduced at the end of this manual), at each iteration the computer checks if either of the following criteria are met:

$$\max_{1 \leq i \leq n} |R_{\alpha_i}^{n+1,m}| \Delta t \leq errorr$$

$$\max_{1 \leq i \leq n} |\delta H_{\alpha_i}^{n+1,m}| \leq errorh$$

Where i ranges over each of the nodes.

Initial conditions

$readic$ 0
 $hydrostaticw$ 1 $hzerow$ -100.0 $hydbotw$ -9.9
 $hydrostatica$ 1 $hzeroa$ 0.0 $hydbota$ 0.1204

$readic$	if $readic \neq 0$ then read the initial pressure distribution from the file $ic.in$. The file contains a list of the water pressures, one entry for each node. Each entry must be separated by white space (a tab, return or space character). The air pressures are set to be zero with this option and are not read from the file.
$hydrostaticw$	if $hydrostaticw \neq 0$ then the water pressure is assumed to have a hydrostatic pressure distribution. The pressure is defined by $h_w(i) = hydbotw - (nn - i) dz \sin(dipangle)$. If $hydrostaticw = 0$, then $h_w = hzerow$.
$hzerow$	If $hydrostaticw = 0$ then the water pressure is assumed initially uniform with pressure given by $hzerow$.
$hydbotw$	The water pressure at the bottom of the column when $hydrostaticw \neq 0$.
$hydrostatica$	if $hydrostatica \neq 0$ then the air pressure is assumed to have a static distribution. The pressure is defined by $h_a(i) = hydbota - (nn - i) dz \sin(dipangle) \times 0.001204$. If $hydrostatica = 0$, then $h_a = hzeroa$.

Appendix

hzeroa If hydrostatica = 0 then the water pressure is assumed initially uniform with pressure given by hzeroa.

hydbota The air pressure at the bottom of the column when hydrostatica != 0.

Flow boundary conditions

```
timestw 1
fluxtw 1 bctw 0.0023 timetw 6000.0
timesta 1
fluxta 0 bcta 0.0 timeta 6000.0
timesbw 1
fluxbw 0 bcbw -9.9 timebw 6000.0
timesba 1
fluxba 0 bcba 0.1204 timeba 6000.0
```

Each boundary condition is specified by 4 variables. The variable names end with two letters that describe the phase and end of the column that the condition applies to. The letter a denotes air, w water, t top and b bottom. For example timestw is the number of time periods for the water boundary condition at the top of the column.

times__ The number of time periods for the boundary condition
For each time period the following three variables are specified (One line per time period).
flux__ flux__ != 0 for a flux condition. Flux = 0 for a fixed pressure condition
bc__ The value of the boundary condition. If it is a flux condition then it has units of (cm/s). If it is a fixed pressure condition it has units of centimeters of water.
time__ the ending time for the boundary condition.

Note: In the above example the bottom boundary condition in the air phase is set so that the air does not move under the force of gravity. It is an air static boundary condition so that

$$bcba = bcta + \rho_a \times \text{length of column}$$

Angle of column

dipangle 1.5707

dipangle the angle of the column with horizontal. For a horizontal column, dipangle=0, for a vertical column, dipangle= $\pi/2$.

Fluid properties

compress 1.0 storativity 2.0e-4

compress If compress = 0.0 then the air is assumed to be incompressible, otherwise the density of air is assumed to be related to the air pressure by the relation

$$\rho_a = 0.001204 \times \left(1.0 + \frac{h_a}{1033.227} \text{compress}\right)$$

storativity elastic storage coefficient. This parameter is set to allow the simulation to apply to the saturated zone.

Ponding

pond 1 hae 14.0

When pond != 0 excess infiltration (infiltration above the infiltration capacity) is allowed to build up as a pond of water at the surface. At each time step the program checks if θ at the top of the column > θ_{ws} . If so, the top boundary conditions are changed. The flux condition on the water phase is changed to a fixed pressure head of water, which is defined to be the difference between the applied flux and the infiltration at the surface. The air is switched to a no flux condition. At every subsequent time step the program then checks to see that the air pressure does not exceed the air entry pressure hae at the surface. If it does, the air boundary condition at the top of the column is switched so that $h_a = h_{ae} + h_w$. (For further discussion of the ponding routine, consult the refer-

ences listed in this manual).

Soil properties

porosity 0.37
 type 1
 thetar 0.0265 thetas 0.312 alpha 0.044 ng 2.2
 kws 0.0042 kas 0.77777777

porosity porosity of sample (note, may be different from θ_{ws} if an imbibition capillary-pressure saturation curve is used.)
 type the soil parameterization type to be used in the simulation. Currently supported values for type are:
 type=1 Touma and Vaucelin Sand
 type=2 Van Genuchten type parameterization. (See Van Genuchten 1980 and Parker 1989)

The type 1 parameterization is described in the paper reprinted at the end of this manual and the type 2 parameterization is described by the following equations:

$$\theta_w = \frac{\theta_{ws} - \theta_{wr}}{|1 + (\alpha h_c)^n|^{1-1/n}} + \theta_{wr}$$

$$K_w = K_{ws} \theta_e^{\frac{1}{2}} \left(1.0 - \left(1.0 - \theta_e^{\frac{1}{m}} \right)^m \right)^2$$

$$K_a = K_{as} (1.0 - \theta_e)^{\frac{1}{2}} \left(1.0 - \theta_e^{\frac{1}{m}} \right)^{2m}$$

where;

$$\theta_e = \frac{\theta - \theta_{wr}}{\theta_{ws} - \theta_{wr}}, \quad m = 1 - 1/n$$

If type = 2 the following values determine the parameterization. These values are always read, but if type=1 they are ignored.

thetar residual water content
 thetas saturated water content
 alpha Van Genuchten alpha parameter
 ng Van Genuchten n parameter
 kws,kas Water and air saturated conductivities (cm/s)

Transport parameters

equilibrium 1 cinit 0
 ctimesw 1
 cfluxtw 0 ctopw 1.0 ctimew 10000.0
 ctimesa 1
 cfluxta 0 ctopa 0.0 ctimea 10000.0
 cbotw 0.0 cbota 0.0
 lambdaw 0.0 lambdaa 0.0 rhos 1.0 kd 0.0 k 0.0 h 0.0
 alphas 1.0 alphaw 1.0 dmoleca 0.0756 dmolecw 0.00001

equilibrium equilibrium = 0 for non- equilibrium transport simulation, otherwise equilibrium transport is assumed.
 cinit cinit = 0 for a uniform initial concentration of contaminant with $c_\alpha = 0$. If cinit != 0 then the initial concentration distribution is determined by reading the file cic.in. Each line of cic.in consists of three entries: depth, c_w and c_a separated by

white space. The node that corresponds to the given depth is set to have initial concentration given by c_w and c_a . All nodes not specified in `cic.in` are assumed to have initial concentration $c_\alpha = 0$.

<code>ctimes_</code>	number of time intervals for the boundary condition
<code>cfluxt_</code>	<code>cfluxt_ = 0</code> for a fixed concentration condition and <code>cflux_ != 0</code> for a flux condition.
<code>ctop_</code>	The value of the boundary condition. <code>ctop_</code> has units of concentration (g/cm^3) if <code>cfluxt_ = 0</code> , and units of phase α flux times concentration ($\frac{\text{g}}{\text{cm}^3} \cdot \frac{\text{cm}}{\text{s}}$).
<code>ctime_</code>	Ending time for the current boundary condition.
<code>cbot_</code>	Bottom boundary conditions are assumed to be of fixed concentration type with value <code>cbot_</code>
<code>lambda_</code>	reaction rate for each phase (units $1/\text{s}$)
<code>rhos</code>	density of the solid phase (units g/cm^3)
<code>kd</code>	distribution coefficient (units cm^3/g). Use <code>rhos</code> and <code>kd</code> to define the retardation coefficient: $R = \left(1 + \frac{\theta_s \rho_s k_d}{\theta_w}\right)$. Values given in the example input file are for an unretarded pollutant.
<code>k</code>	Kinetic Mass transfer coefficient (cm/s) (see Cho and Jaffe, 1990)
<code>h</code>	Henry's Constant
<code>alpha_</code>	dispersivity (cm)
<code>dmolec_</code>	molecular diffusion for each phase. (The example file contains typical values for TCE)

Printing control

```
pmatrix 0 reswrite 0 flush 1
vprint 1 nvprint 10
tvprint
600. 1200. 1800. 2400. 3000. 3600. 4200. 4800. 5400. 6000.
```

<code>pmatrix</code>	A debugging tool. If <code>pmatrix!=0</code> , the Finite element matrices are printed in the output file
<code>rewrite</code>	<code>rewrite != 0</code> to print the maximum residual at each iteration. This option can be used to see how fast the non-linear iteration scheme converges
<code>flush</code>	C stores output in a memory buffer, collecting the output until the buffer fills and then writes the information to the output files. This feature of C allows programs that are intensive in output to run much faster. However, if you stop the program before it is finished or it crashes the output is lost. Setting <code>flush = 1</code> causes the program to flush the output buffers at the end of each time step. If you want the program to run faster, set <code>flush = 0</code> .
<code>vprint</code>	<code>vprint != 0</code> if printing is desired at fixed times given by the array <code>tvprint</code> . This option is useful if variable sized time steps are used as it forces the program to print output at particular times.
<code>nvprint</code>	number of times to print the output
<code>tvprint</code>	One line with entries separated by spaces or tabs, containing the times to print the output.

8. Example input files included with code

Several example files are included with the code. The solutions to the flow equation are discussed in the paper that is referenced on the cover and in Touma and Vaucelin (1986). The transport results are discussed in Celia, Sweed and Binning (1993).

83open.in

This is the input file described above

83closed.in

As 83 open.in but with a no flux boundary in the air and water phases at the bottom of the column.

20open.in

As 83open.in but with a flux of 20cm/h at the top of the column rather than 8.3 cm/h. As the flux is higher than the saturated water conductivity, the water ponds on the surface.

20closed.in

As 20open.in but with a no flow condition at the bottom of the column.

wonly.in

In this example a salt tracer is followed as it is carried by the water from the middle of the column. As the salt does not partition into the air phase only transport in the water phase is considered (this is achieved in the code by setting $H=0$ and equilibrium = 1 so that $c_a = 0$. This is equivalent to only solving the transport equation for the water phase). The flow of air and water are as described in example 20closed.in. The salt tracer is added at the nodes at 32 and 36 cm with a concentration of 1.0. The boundary conditions of the water contaminant transport equation are $c_w = 0.0$ at both ends of the column. No boundary conditions are needed for the air phase as the air equation is degenerate. Note that this example reads the file cic.in to determine the initial distribution of contaminant.

eq.in

As wonly.in but with equilibrium partitioning between the air and water phases. Henry's constant is chosen as that for TCE. Here equilibrium = 1 and $H=0.392$.

noneq.in

As wonly.in but with non equilibrium partitioning between the phases.

9. Output files

The program generates a variety of output files. The major output file is:

2p.out General output file. See the section "Sample Output" for an example. Use this file to check input variables and see results in numerical form.

The program also generates a variety of graphics files. These files are generated in files.c. Within the program, variables and functions that deal with output to files for use in graphics usually contain the letter x in their name (The program was developed with X windows graphics).

Note that for the xgraph files (those ending in x) the negative of the depth is written rather than the depth. This is so that the origin appears at the top of the graph and the bottom of the simulated column is at the bottom of the graph. Examples of these plots are given later in the manual for the input file discussed above.

p.x	Pressures of water and air. At each output time step (controlled by nprint or vprint), the program writes the pressure of each phase. The format of the file is that at each output time the time in minutes is printed followed by one entry per node specifying the pressure and depth of that node.
theta.x	moisture content at each output time step.
qw.x	Water flux at each output time step.
qa.x	Air flux at each output time step.
infil.x	Cumulative infiltration with time. At each time step the amount of water that has infiltrated through the surface (cm water) is written to the file.
massbal.x	At each time step the mass balance of the water and air in that order are written to the file in the format time (minutes), massbal_.

Appendix

dt.x	Time step size at each time step.
cw.x	Water concentration at each output time step
ca.x	Air concentration at each output time step
iter.x	Number of iterations needed for convergence at each time step.
graphics.out	Graphics output.

10. Sample Output

```
*****
*   TWO PHASE FLOW AND TRANSPORT CODE   *
*                                         *
*   Based on the work of Celia and Binning *
*   Appeared in Water Resources Research Oct 1992 *
*                                         *
*   Code written by Philip Binning Feb 1992 *
*****
```

```
*****
*   Input Parameters *
*****
```

MESH PARAMETERS

number of nodes nn 26
Node Spacing dz 4.000000

TIME STEPPING PARAMETERS

Time step size dt 10.000000
Number of time steps in simulation timetot 6000
Number of time steps between printing steps nprint 6000
Maximum time of simulation maxtime 6000.000000
Minimum Iterations before increasing dt itmin 10
Maximum Iterations before decreasing dt itmax 15
Time step decreased by dtdec if iterations > itmax 0.950000
Time step increased by dtinc if iterations < itmin 1.050000

ERROR TOLERANCES

Maximum number of iterations per time step maxiter 40
Maximum error for convergence in residual, error 0.000100
Maximum error for convergence in head, errorh 0.100000

INITIAL CONDITIONS

Read initial conditions if readic != 0: readic = 0
Hydrostatic initial conditions if hydrostatic !=0: hydrostaticw = 1
Value for uniform initial condition hzerow -100.000000
Water Pressure at bottom of column for hydrostatic
initial condition hydbotw = -9.900000
Hydrostatic initial conditions if hydrostatic !=0: hydrostatica = 1
Value for uniform initial condition hzeroa 0.000000
Air Pressure at bottom of column for hydrostatic
initial condition hydbota = 0.120400

BOUNDARY CONDITIONS

Number of time intervals for water at top timestw 1
bc type (1 for flux) 1 value 0.002300 ending time 6000.000000

Number of time intervals for air at top timesta 1
bc type (1 for flux) 0 value 0.000000 ending time 6000.000000

No. of time intervals for water at bottom timesbw 1
bc type (1 for flux) 0 value -9.900000 ending time 6000.000000

Number of time intervals for air at bottom timesba 1
 bc type (1 for flux) 0 value 0.120400 ending time 6000.000000

ANGLE OF COLUMN

Angle of column dipangle 1.570700

COMPRESSIBILITY

compress (=1 for compressible air) 1.000000
 storativity 0.000200

PONDING

ponding allowed at surface (=1 for true) 1
 Air entry pressure hae = 14.000000(for use in ponding routine)

MATERIAL PARAMETERS

POROSITY

porosity 0.370000
 Material is touma and Vauclin sand

CONTAMINANT TRANSPORT VARIABLES

Equilibrium partitioning between phases(=1 for true) 1
 Note: if equilibrium partitioning then only use water parameters
 Read concentration initial conditions (=1 for true) 0

Number of time intervals for water at top ctimesw 1
 bc type (1 for flux) 0 value 1.000000 ending time 10000.000000

Number of time intervals for air at top ctimesa 1
 bc type (1 for flux) 0 value 0.000000 ending time 10000.000000
 Concentration in air at bottom cbota 0.000000
 Concentration in water at bottom cbotw 0.000000

Chemical reactivity of water lambdaw 0.000000
 Chemical reactivity of air lambdawa 0.000000
 density of solid phase rhos 1.000000
 distribution coefficient kd 0.000000
 Mass Transfer coefficient 0.000000
 Henry's Constant 0.000000
 Dispersivity in air alphaa 1.000000
 Dispersivity in water alphaw 1.000000
 Molecular Diffusion in air dmoleca 0.075600
 Molecular Diffusion in water dmolecw 0.000010

PRINTING CONTROL

print matrix (=1) for printing: pmatrix = 0
 reswrite =1 for printing residuals: reswrite= 0
 flush=0 to allow buffering of output : flush= 1
 Use buffering to speed up program. Turn it off for debugging
 vprint (=1) for output at tvprint steps: vprint = 1
 Number of steps at which variable printing occurs nvprint 10
 Times at which printing is to occur
 600.0 1200.0 1800.0 2400.0 3000.0 3600.0 4200.0 4800.0 5400.0 6000.0

 * Initial Conditions *

node	z	water head	air head	theta	cw	ca
1	0.00	-109.9000	0.0000	0.0682	0.000000	0.000000
2	-4.00	-105.9000	0.0048	0.0700	0.000000	0.000000
3	-8.00	-101.9000	0.0096	0.0720	0.000000	0.000000
4	-12.00	-97.9000	0.0144	0.0742	0.000000	0.000000
5	-16.00	-93.9000	0.0193	0.0766	0.000000	0.000000

Appendix

6	-20.00	-89.9000	0.0241	0.0792	0.000000	0.000000
7	-24.00	-85.9000	0.0289	0.0820	0.000000	0.000000
8	-28.00	-81.9000	0.0337	0.0851	0.000000	0.000000
9	-32.00	-77.9000	0.0385	0.0885	0.000000	0.000000
10	-36.00	-73.9000	0.0433	0.0923	0.000000	0.000000
11	-40.00	-69.9000	0.0482	0.0966	0.000000	0.000000
12	-44.00	-65.9000	0.0530	0.1013	0.000000	0.000000
13	-48.00	-61.9000	0.0578	0.1066	0.000000	0.000000
14	-52.00	-57.9000	0.0626	0.1126	0.000000	0.000000
15	-56.00	-53.9000	0.0674	0.1194	0.000000	0.000000
16	-60.00	-49.9000	0.0722	0.1271	0.000000	0.000000
17	-64.00	-45.9000	0.0771	0.1360	0.000000	0.000000
18	-68.00	-41.9000	0.0819	0.1462	0.000000	0.000000
19	-72.00	-37.9000	0.0867	0.1580	0.000000	0.000000
20	-76.00	-33.9000	0.0915	0.1716	0.000000	0.000000
21	-80.00	-29.9000	0.0963	0.1873	0.000000	0.000000
22	-84.00	-25.9000	0.1011	0.2052	0.000000	0.000000
23	-88.00	-21.9000	0.1060	0.2253	0.000000	0.000000
24	-92.00	-17.9000	0.1108	0.2470	0.000000	0.000000
25	-96.00	-13.9000	0.1156	0.2690	0.000000	0.000000
26	-100.00	-9.9000	0.1204	0.2890	0.000000	0.000000

Timestep number 29 Time 600.000000 dt= 39.201291 iterations 4

mass balance for water 1.000197 cumulative mass balance for water 1.000253
mass balance for air 1.000020 cumulative mass balance for air 1.000126

node	depth	water head	air head	water content	cw	ca
1	0.0	-16.6533	0.0000	0.254552	1.0000	0.0000
2	4.0	-22.4744	0.2016	0.221768	0.7650	0.0000
3	8.0	-39.6060	0.2527	0.152238	0.3174	0.0000
4	12.0	-86.4063	0.2583	0.081453	0.0195	0.0000
5	16.0	-93.5910	0.2610	0.076624	0.0000	0.0000
6	20.0	-89.6741	0.2638	0.079156	0.0000	0.0000
7	24.0	-85.6759	0.2664	0.081984	0.0000	0.0000
8	28.0	-81.6773	0.2690	0.085093	0.0000	0.0000
9	32.0	-77.6788	0.2715	0.088525	0.0000	0.0000
10	36.0	-73.6805	0.2738	0.092326	0.0000	0.0000
11	40.0	-69.6823	0.2760	0.096556	0.0000	0.0000
12	44.0	-65.6844	0.2781	0.101282	0.0000	0.0000
13	48.0	-61.6867	0.2799	0.106590	0.0000	0.0000
14	52.0	-57.6893	0.2815	0.112578	0.0000	0.0000
15	56.0	-53.6923	0.2827	0.119369	0.0000	0.0000
16	60.0	-49.6958	0.2835	0.127110	0.0000	0.0000
17	64.0	-45.7000	0.2838	0.135976	0.0000	0.0000
18	68.0	-41.7052	0.2833	0.146175	0.0000	0.0000
19	72.0	-37.7121	0.2818	0.157943	0.0000	0.0000
20	76.0	-33.7224	0.2790	0.171535	0.0000	0.0000
21	80.0	-29.7391	0.2741	0.187184	0.0000	0.0000
22	84.0	-25.7649	0.2662	0.205036	0.0000	0.0000
23	88.0	-21.7992	0.2534	0.225030	0.0000	0.0000
24	92.0	-17.8368	0.2324	0.246681	0.0000	0.0000
25	96.0	-13.8718	0.1953	0.268752	0.0000	0.0000
26	100.0	-9.9000	0.1204	0.288996	0.0000	0.0000

Timestep number 41 Time 1200.000000 dt= 67.047512 iterations 5

mass balance for water 1.000110 cumulative mass balance for water 1.000020
mass balance for air 0.999849 cumulative mass balance for air 1.000129

node	depth	water head	air head	water content	cw	ca
1	0.0	-13.5063	0.0000	0.271748	1.0000	0.0000
2	4.0	-14.9307	0.3409	0.262196	0.9700	0.0000
3	8.0	-17.8179	0.5573	0.244984	0.7572	0.0000
4	12.0	-24.7261	0.6524	0.208175	0.4257	0.0000

Sample Output

5	16.0	-44.5071	0.6699	0.137921	0.1345	0.0000
6	20.0	-83.4637	0.6684	0.083355	0.0045	0.0000
7	24.0	-85.2347	0.6674	0.082014	0.0000	0.0000
8	28.0	-81.3006	0.6663	0.085077	0.0000	0.0000
9	32.0	-77.3052	0.6650	0.088507	0.0000	0.0000
10	36.0	-73.3096	0.6633	0.092308	0.0000	0.0000
11	40.0	-69.3145	0.6612	0.096536	0.0000	0.0000
12	44.0	-65.3199	0.6587	0.101262	0.0000	0.0000
13	48.0	-61.3261	0.6556	0.106568	0.0000	0.0000
14	52.0	-57.3332	0.6518	0.112555	0.0000	0.0000
15	56.0	-53.3414	0.6471	0.119345	0.0000	0.0000
16	60.0	-49.3511	0.6412	0.127083	0.0000	0.0000
17	64.0	-45.3635	0.6339	0.135943	0.0000	0.0000
18	68.0	-41.3807	0.6245	0.146129	0.0000	0.0000
19	72.0	-37.4079	0.6126	0.157860	0.0000	0.0000
20	76.0	-33.4530	0.5968	0.171358	0.0000	0.0000
21	80.0	-29.5213	0.5758	0.186832	0.0000	0.0000
22	84.0	-25.6083	0.5467	0.204447	0.0000	0.0000
23	88.0	-21.7004	0.5047	0.224228	0.0000	0.0000
24	92.0	-17.7839	0.4406	0.245820	0.0000	0.0000
25	96.0	-13.8508	0.3327	0.268125	0.0000	0.0000
26	100.0	-9.9000	0.1204	0.288996	0.0000	0.0000

Timestep number 49 Time 1800.000000 dt= 94.342582 iterations 5

mass balance for water 1.000028 cumulative mass balance for water 0.999895
mass balance for air 0.999943 cumulative mass balance for air 1.000178

node	depth	water head	air head	water content	cw	ca
1	0.0	-12.2766	0.0000	0.278145	1.0000	0.0000
2	4.0	-12.7702	0.3562	0.273753	1.0094	0.0000
3	8.0	-13.7240	0.6395	0.267152	0.9493	0.0000
4	12.0	-15.4957	0.8413	0.256308	0.7594	0.0000
5	16.0	-19.0579	0.9564	0.235965	0.4858	0.0000
6	20.0	-27.6886	0.9936	0.192900	0.2261	0.0000
7	24.0	-51.6086	0.9930	0.121914	0.0510	0.0000
8	28.0	-78.8517	0.9868	0.086860	0.0007	0.0000
9	32.0	-76.9710	0.9822	0.088522	0.0000	0.0000
10	36.0	-73.0102	0.9773	0.092293	0.0000	0.0000
11	40.0	-69.0182	0.9717	0.096520	0.0000	0.0000
12	44.0	-65.0265	0.9655	0.101245	0.0000	0.0000
13	48.0	-61.0359	0.9583	0.106551	0.0000	0.0000
14	52.0	-57.0468	0.9501	0.112536	0.0000	0.0000
15	56.0	-53.0598	0.9405	0.119323	0.0000	0.0000
16	60.0	-49.0759	0.9292	0.127056	0.0000	0.0000
17	64.0	-45.0985	0.9157	0.135904	0.0000	0.0000
18	68.0	-41.1345	0.8992	0.146051	0.0000	0.0000
19	72.0	-37.1952	0.8786	0.157691	0.0000	0.0000
20	76.0	-33.2893	0.8525	0.171024	0.0000	0.0000
21	80.0	-29.4125	0.8184	0.186273	0.0000	0.0000
22	84.0	-25.5470	0.7724	0.203668	0.0000	0.0000
23	88.0	-21.6715	0.7074	0.223318	0.0000	0.0000
24	92.0	-17.7727	0.6090	0.244948	0.0000	0.0000
25	96.0	-13.8477	0.4447	0.267537	0.0000	0.0000
26	100.0	-9.9000	0.1204	0.288996	0.0000	0.0000

Timestep number 55 Time 2400.000000 dt= 120.407698 iterations 6

mass balance for water 0.999862 cumulative mass balance for water 0.999914
mass balance for air 1.000088 cumulative mass balance for air 1.000133

node	depth	water head	air head	water content	cw	ca
1	0.0	-11.6929	0.0000	0.281076	1.0000	0.0000
2	4.0	-11.8314	0.3270	0.278744	1.0074	0.0000
3	8.0	-12.1818	0.6136	0.275479	1.0047	0.0000

Appendix

4	12.0	-12.8477	0.8522	0.270719	0.9338	0.0000
5	16.0	-14.0285	1.0350	0.263338	0.7640	0.0000
6	20.0	-16.1738	1.1553	0.250794	0.5287	0.0000
7	24.0	-20.5502	1.2113	0.226568	0.2949	0.0000
8	28.0	-31.1368	1.2171	0.177737	0.1153	0.0000
9	32.0	-56.9675	1.2071	0.112254	0.0166	0.0000
10	36.0	-71.8957	1.1977	0.093199	0.0001	0.0000
11	40.0	-68.7891	1.1896	0.096533	0.0000	0.0000
12	44.0	-64.8203	1.1807	0.101234	0.0000	0.0000
13	48.0	-60.8328	1.1707	0.106538	0.0000	0.0000
14	52.0	-56.8469	1.1593	0.112521	0.0000	0.0000
15	56.0	-52.8640	1.1463	0.119305	0.0000	0.0000
16	60.0	-48.8873	1.1311	0.127029	0.0000	0.0000
17	64.0	-44.9235	1.1131	0.135850	0.0000	0.0000
18	68.0	-40.9854	1.0915	0.145933	0.0000	0.0000
19	72.0	-37.0855	1.0649	0.157450	0.0000	0.0000
20	76.0	-33.2250	1.0315	0.170608	0.0000	0.0000
21	80.0	-29.3868	0.9883	0.185673	0.0000	0.0000
22	84.0	-25.5450	0.9307	0.202931	0.0000	0.0000
23	88.0	-21.6790	0.8496	0.222536	0.0000	0.0000
24	92.0	-17.7806	0.7276	0.244247	0.0000	0.0000
25	96.0	-13.8519	0.5240	0.267085	0.0000	0.0000
26	100.0	-9.9000	0.1204	0.288996	0.0000	0.0000

Timestep number 60 Time 3000.000000 dt= 146.356309 iterations 6

mass balance for water 0.999938 cumulative mass balance for water 0.999949
mass balance for air 1.000029 cumulative mass balance for air 1.000088

node	depth	water head	air head	water content	cw	ca
1	0.0	-11.4103	0.0000	0.282468	1.0000	0.0000
2	4.0	-11.3890	0.2871	0.281160	1.0022	0.0000
3	8.0	-11.4802	0.5525	0.279379	1.0097	0.0000
4	12.0	-11.7263	0.7908	0.276916	0.9968	0.0000
5	16.0	-12.1957	0.9959	0.273410	0.9224	0.0000
6	20.0	-13.0079	1.1613	0.268202	0.7694	0.0000
7	24.0	-14.3974	1.2809	0.259955	0.5621	0.0000
8	28.0	-16.9080	1.3500	0.245634	0.3492	0.0000
9	32.0	-22.0828	1.3701	0.217766	0.1736	0.0000
10	36.0	-34.2593	1.3592	0.165793	0.0561	0.0000
11	40.0	-57.7971	1.3434	0.110748	0.0048	0.0000
12	44.0	-64.1772	1.3309	0.101855	0.0000	0.0000
13	48.0	-60.6733	1.3188	0.106554	0.0000	0.0000
14	52.0	-56.7076	1.3052	0.112511	0.0000	0.0000
15	56.0	-52.7301	1.2897	0.119288	0.0000	0.0000
16	60.0	-48.7622	1.2718	0.126997	0.0000	0.0000
17	64.0	-44.8164	1.2506	0.135778	0.0000	0.0000
18	68.0	-40.9079	1.2254	0.145779	0.0000	0.0000
19	72.0	-37.0453	1.1946	0.157169	0.0000	0.0000
20	76.0	-33.2185	1.1561	0.170180	0.0000	0.0000
21	80.0	-29.4017	1.1067	0.185121	0.0000	0.0000
22	84.0	-25.5671	1.0410	0.202310	0.0000	0.0000
23	88.0	-21.6986	0.9490	0.221917	0.0000	0.0000
24	92.0	-17.7934	0.8106	0.243717	0.0000	0.0000
25	96.0	-13.8576	0.5797	0.266752	0.0000	0.0000
26	100.0	-9.9000	0.1204	0.288996	0.0000	0.0000

Timestep number 64 Time 3600.000000 dt= 161.357831 iterations 8

mass balance for water 1.000071 cumulative mass balance for water 0.999956
mass balance for air 0.999938 cumulative mass balance for air 1.000070

node	depth	water head	air head	water content	cw	ca
1	0.0	-11.2806	0.0000	0.283099	1.0000	0.0000
2	4.0	-11.1851	0.2484	0.282354	1.0000	0.0000

3	8.0	-11.1532	0.4857	0.281344	1.0045	0.0000
4	12.0	-11.2059	0.7081	0.279975	1.0087	0.0000
5	16.0	-11.3736	0.9115	0.278101	0.9882	0.0000
6	20.0	-11.7028	1.0913	0.275486	0.9138	0.0000
7	24.0	-12.2688	1.2421	0.271724	0.7748	0.0000
8	28.0	-13.2057	1.3585	0.266063	0.5895	0.0000
9	32.0	-14.7799	1.4354	0.256983	0.3945	0.0000
10	36.0	-17.6100	1.4702	0.241087	0.2247	0.0000
11	40.0	-23.3607	1.4673	0.210867	0.1009	0.0000
12	44.0	-35.8414	1.4458	0.160209	0.0273	0.0000
13	48.0	-53.7096	1.4247	0.117308	0.0017	0.0000
14	52.0	-56.1652	1.4079	0.113216	0.0000	0.0000
15	56.0	-52.6124	1.3905	0.119318	0.0000	0.0000
16	60.0	-48.6809	1.3706	0.126960	0.0000	0.0000
17	64.0	-44.7578	1.3472	0.135688	0.0000	0.0000
18	68.0	-40.8791	1.3194	0.145601	0.0000	0.0000
19	72.0	-37.0471	1.2857	0.156878	0.0000	0.0000
20	76.0	-33.2423	1.2437	0.169780	0.0000	0.0000
21	80.0	-29.4341	1.1900	0.184644	0.0000	0.0000
22	84.0	-25.5974	1.1187	0.201805	0.0000	0.0000
23	88.0	-21.7210	1.0190	0.221436	0.0000	0.0000
24	92.0	-17.8068	0.8693	0.243318	0.0000	0.0000
25	96.0	-13.8634	0.6193	0.266506	0.0000	0.0000
26	100.0	-9.9000	0.1204	0.288996	0.0000	0.0000

Timestep number 68 Time 4200.000000 dt= 169.425722 iterations 7

mass balance for water 1.000027 cumulative mass balance for water 0.999959
mass balance for air 0.999977 cumulative mass balance for air 1.000059

node	depth	water head	air head	water content	cw	ca
1	0.0	-11.2298	0.0000	0.283345	1.0000	0.0000
2	4.0	-11.1022	0.2140	0.282926	0.9996	0.0000
3	8.0	-11.0113	0.4224	0.282353	1.0009	0.0000
4	12.0	-10.9685	0.6231	0.281577	1.0057	0.0000
5	16.0	-10.9893	0.8134	0.280530	1.0060	0.0000
6	20.0	-11.0953	0.9903	0.279112	0.9809	0.0000
7	24.0	-11.3179	1.1501	0.277168	0.9084	0.0000
8	28.0	-11.7052	1.2886	0.274446	0.7813	0.0000
9	32.0	-12.3354	1.4014	0.270522	0.6134	0.0000
10	36.0	-13.3462	1.4838	0.264615	0.4329	0.0000
11	40.0	-15.0084	1.5320	0.255179	0.2690	0.0000
12	44.0	-17.9335	1.5445	0.238899	0.1412	0.0000
13	48.0	-23.6446	1.5272	0.209181	0.0564	0.0000
14	52.0	-34.9339	1.4977	0.153030	0.0125	0.0000
15	56.0	-47.6516	1.4704	0.128911	0.0006	0.0000
16	60.0	-48.1738	1.4469	0.127857	0.0000	0.0000
17	64.0	-44.6844	1.4216	0.135686	0.0000	0.0000
18	68.0	-40.8713	1.3918	0.145426	0.0000	0.0000
19	72.0	-37.0671	1.3558	0.156597	0.0000	0.0000
20	76.0	-33.2755	1.3112	0.169418	0.0000	0.0000
21	80.0	-29.4686	1.2542	0.184239	0.0000	0.0000
22	84.0	-25.6254	1.1787	0.201395	0.0000	0.0000
23	88.0	-21.7401	1.0731	0.221057	0.0000	0.0000
24	92.0	-17.8177	0.9146	0.243008	0.0000	0.0000
25	96.0	-13.8679	0.6498	0.266316	0.0000	0.0000
26	100.0	-9.9000	0.1204	0.288996	0.0000	0.0000

Timestep number 72 Time 4800.000000 dt= 177.897009 iterations 6

mass balance for water 1.000005 cumulative mass balance for water 0.999962
mass balance for air 0.999991 cumulative mass balance for air 1.000050

node	depth	water head	air head	water content	cw	ca
1	0.0	-11.2225	0.0000	0.283381	1.0000	0.0000

Appendix

2	4.0	-11.0851	0.1843	0.283154	0.9998	0.0000
3	8.0	-10.9688	0.3661	0.282835	0.9997	0.0000
4	12.0	-10.8801	0.5441	0.282400	1.0019	0.0000
5	16.0	-10.8274	0.7167	0.281811	1.0059	0.0000
6	20.0	-10.8219	0.8821	0.281021	1.0027	0.0000
7	24.0	-10.8790	1.0378	0.279961	0.9748	0.0000
8	28.0	-11.0198	1.1812	0.278529	0.9051	0.0000
9	32.0	-11.2751	1.3091	0.276570	0.7883	0.0000
10	36.0	-11.6917	1.4180	0.273840	0.6347	0.0000
11	40.0	-12.3446	1.5037	0.269926	0.4667	0.0000
12	44.0	-13.3629	1.5625	0.264094	0.3086	0.0000
13	48.0	-14.9916	1.5910	0.254945	0.1789	0.0000
14	52.0	-17.7461	1.5884	0.239687	0.0866	0.0000
15	56.0	-22.7449	1.5604	0.213461	0.0313	0.0000
16	60.0	-31.4485	1.5215	0.175375	0.0063	0.0000
17	64.0	-39.9331	1.4839	0.147756	0.0003	0.0000
18	68.0	-40.1661	1.4491	0.147204	0.0000	0.0000
19	72.0	-36.9862	1.4107	0.156677	0.0000	0.0000
20	76.0	-33.2915	1.3639	0.169173	0.0000	0.0000
21	80.0	-29.4975	1.3044	0.183916	0.0000	0.0000
22	84.0	-25.6497	1.2255	0.201064	0.0000	0.0000
23	88.0	-21.7563	1.1154	0.220754	0.0000	0.0000
24	92.0	-17.8267	0.9500	0.242762	0.0000	0.0000
25	96.0	-13.8716	0.6738	0.266166	0.0000	0.0000
26	100.0	-9.9000	0.1204	0.288996	0.0000	0.0000

Timestep number 76 Time 5400.000000 dt= 186.791859 iterations 5

mass balance for water 0.999992 cumulative mass balance for water 0.999966
mass balance for air 0.999996 cumulative mass balance for air 1.000043

node	depth	water head	air head	water content	cw	ca
1	0.0	-11.2379	0.0000	0.283306	1.0000	0.0000
2	4.0	-11.1025	0.1591	0.283192	1.0000	0.0000
3	8.0	-10.9790	0.3173	0.283023	0.9997	0.0000
4	12.0	-10.8713	0.4738	0.282786	1.0000	0.0000
5	16.0	-10.7840	0.6277	0.282461	1.0026	0.0000
6	20.0	-10.7234	0.7779	0.282022	1.0053	0.0000
7	24.0	-10.6974	0.9230	0.281435	0.9993	0.0000
8	28.0	-10.7165	1.0613	0.280654	0.9697	0.0000
9	32.0	-10.7952	1.1909	0.279614	0.9032	0.0000
10	36.0	-10.9530	1.3091	0.278218	0.7953	0.0000
11	40.0	-11.2180	1.4133	0.276328	0.6540	0.0000
12	44.0	-11.6319	1.5003	0.273722	0.4970	0.0000
13	48.0	-12.2591	1.5665	0.270047	0.3450	0.0000
14	52.0	-13.2053	1.6085	0.264703	0.2150	0.0000
15	56.0	-14.6546	1.6234	0.256635	0.1172	0.0000
16	60.0	-16.9433	1.6104	0.243995	0.0532	0.0000
17	64.0	-20.6442	1.5731	0.224164	0.0182	0.0000
18	68.0	-26.1560	1.5215	0.197382	0.0038	0.0000
19	72.0	-31.2605	1.4662	0.176302	0.0003	0.0000
20	76.0	-31.7758	1.4100	0.174560	0.0000	0.0000
21	80.0	-29.1270	1.3458	0.185269	0.0000	0.0000
22	84.0	-25.5540	1.2633	0.201333	0.0000	0.0000
23	88.0	-21.7303	1.1492	0.220714	0.0000	0.0000
24	92.0	-17.8194	0.9782	0.242647	0.0000	0.0000
25	96.0	-13.8696	0.6927	0.266073	0.0000	0.0000
26	100.0	-9.9000	0.1204	0.288996	0.0000	0.0000

Timestep number 80 Time 6000.000000 dt= 0.000000 iterations 3

mass balance for water 0.999991 cumulative mass balance for water 0.999969
mass balance for air 1.000008 cumulative mass balance for air 1.000037

node	depth	water head	air head	water content	cw	ca
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Sample Output

1	0.0	-11.2674	0.0000	0.283163	1.0000	0.0000
2	4.0	-11.1415	0.1357	0.283116	1.0000	0.0000
3	8.0	-11.0221	0.2713	0.283037	0.9998	0.0000
4	12.0	-10.9116	0.4065	0.282917	0.9997	0.0000
5	16.0	-10.8125	0.5406	0.282746	1.0005	0.0000
6	20.0	-10.7284	0.6731	0.282510	1.0029	0.0000
7	24.0	-10.6637	0.8030	0.282191	1.0042	0.0000
8	28.0	-10.6238	0.9295	0.281766	0.9958	0.0000
9	32.0	-10.6161	1.0513	0.281203	0.9653	0.0000
10	36.0	-10.6498	1.1668	0.280462	0.9018	0.0000
11	40.0	-10.7373	1.2743	0.279485	0.8016	0.0000
12	44.0	-10.8954	1.3717	0.278193	0.6711	0.0000
13	48.0	-11.1469	1.4565	0.276472	0.5243	0.0000
14	52.0	-11.5241	1.5259	0.274153	0.3787	0.0000
15	56.0	-12.0738	1.5768	0.270982	0.2501	0.0000
16	60.0	-12.8644	1.6063	0.266571	0.1485	0.0000
17	64.0	-13.9966	1.6114	0.260343	0.0774	0.0000
18	68.0	-15.6068	1.5907	0.251527	0.0341	0.0000
19	72.0	-17.8144	1.5445	0.239553	0.0119	0.0000
20	76.0	-20.4438	1.4768	0.225726	0.0029	0.0000
21	80.0	-22.4708	1.3925	0.215682	0.0004	0.0000
22	84.0	-22.4725	1.2921	0.216182	0.0000	0.0000
23	88.0	-20.4304	1.1650	0.227449	0.0000	0.0000
24	92.0	-17.2855	0.9847	0.245566	0.0000	0.0000
25	96.0	-13.6835	0.6925	0.267085	0.0000	0.0000
26	100.0	-9.9000	0.1204	0.288996	0.0000	0.0000

11. Graphics Output

p.x

Pressure of Air and Water with time

Please note that for plotting purposes these x graphs are labelled with negative depth. In the program depth is **positive** down.

theta.x

qw.x

Note that the flux is plotted in the middle of the elements (between the nodes). The flux at 0 (not plotted) is 0.0023 cm/s as defined by the boundary condition. The graph shows that the water is moving down behind the infiltration front but is stationary where the moisture content is low.

qa.x

The air is moving down (flux positive) in front of the infiltrating front, but is moving up behind the front. This is because the infiltrating water increases the air pressure in front of the front causing a pressure gradient to form towards both ends of the column. This example shows that even in situations where the air is free to escape through the bottom of the column, there will be some movement of air towards the surface. The plot on the cover of this manual shows the air movement as particle tracks which shows that about 1/3 of the air escapes through the top of the column.

inflt.x

This graph is linear as the flux rate (which equals the slope of the graph) is constant.

massbal.x

Both the mass balance of air and water are shown on the graph. The graphing package only prints two decimal places on the y-axis. A discussion of this graph can be found in Celia and Binning where the same figure is plotted with different line types for the air and water.

dt.x

Time step size as a function of time step. Note that the time step increases whenever the number of non linear iterations is less than 10 (see iter.x). The spikes in the graph are due to the program taking smaller time steps in order to arrive exactly at the times when the user requested printing of output. After printing the time step is restored to its previous size.

iter.x

Generally the number of iterations increases as the time step size increases. The number of iterations decrease for a given time step size as the non linearities in the equation become weaker (i.e. as the infiltrating front becomes less steep (the pressure changes less rapidly with depth)). The variable time step option of the program is controlled by checking the number of iterations the non linear iteration scheme takes to converge.

cw.x

The concentration plume lags behind the infiltrating water front because the clean water that was in the column initially (as the initial moisture content) gets pushed in front of the infiltrating contaminated water.

ca.x

The contaminant in this problem is salt so there is no contaminant in the air phase. (Henry's constant $H=0.0$)

12. Errors

Input file

If you encounter an error while using the program check the input file carefully. Most errors are made by setting it up incorrectly. If the program does crash because the input is incorrect, check the file 2p.out to make sure that you have set up the input file correctly. The program writes the input to the output file as it is read, so this is the best place to start. If everything seems ok and the program still will not run, compare your input file with the example input files that come with the code. These files have been tested and should run correctly.

Memory

The program dynamically allocates memory using the C functions malloc and calloc. These are included in the program using the header file 'myvector.h'. If there is not enough memory to run the code the computer will print out the message 'cannot allocate space' and then crash. If this happens reduce the size of the problem you are considering.

13. References

- Binning, Philip, Modeling unsaturated zone flow and contaminant transport in the air and water phases, Ph.D. thesis, Department of Civil Engineering and Operations Research, Princeton University, Princeton, New Jersey, January 1994.
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- van Genuchten, M.Th., A closed form for predicting the hydraulic conductivity of soils, *Soil Science Society of America*, **44**, 892-898, 1980.

14. Program structure

15. Compilation

The code has been compiled and run on the following systems: IBM PC, IBM RS 6000, DEC 3100, IRIS Indigo. It is written in ANSI Standard C and is fully portable.

Compiling on the IBM PC

The code has been compiled on the IBM PC using a typical DOS compiler for the C language.

Compiling with a UNIX machine

The program can be compiled on a UNIX machine by using the following makefile

```
CFLAGS = -lm -O
objects = 2p.o files.o banded.o functions.o transport.o
edit : $(objects)
        cc -o 2p $(objects) $(CFLAGS)
2p.o : myvector.h files.h functions.h banded.h
files.o : files.h myvector.h
banded.o : banded.h
functions.o : functions.h
transport.o : transport.h myvector.h functions.h banded.h
```

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11. ABSTRACT (200 words or less)

A numerical model of multiphase air-water flow and contaminant transport in the unsaturated zone is presented. The multiphase flow equations are solved using the two-pressure, mixed form of the equations with a modified Picard linearization of the equations and a finite element spatial approximation. A volatile contaminant is assumed to be transported in either phase, or in both phases simultaneously. The contaminant partitions between phases with an equilibrium distribution given by Henry's Law or via kinetic mass transfer. The transport equations are solved using a Galerkin finite element method with reduced integration to lump the resultant matrices. The numerical model is applied to published experimental studies to examine the behavior of the air phase and associated contaminant movement under water infiltration. The model is also used to evaluate a hypothetical design for a low-level radioactive waste disposal facility. The model has been developed in both one and two dimensions; documentation and computer codes are available for the one-dimensional flow and transport model.

12. KEY WORDS/DESCRIPTORS (List words or phrases that will assist researchers in locating the report.)

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