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IDENTIFICATION AND COMPILATION OF UNSATURATED/VADOSE ZONE MODELS

by

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FOREWORD

EPA is charged by Congress to protect the Nation's land, air, and water systems. Under a mandate of national environmental laws focused on air and water quality, solid waste management and the control of toxic substances, pesticides, noise and radiation, the Agency strives to formulate and implement actions which lead to a compatible balance between human activities and the ability of natural systems to support and nurture life.

The Robert S. Kerr Environmental Research Laboratory is the Agency's center of expertise for investigation of the soil and subsurface environment. Personnel at the laboratory are responsible for management of research programs to: (a) determine the fate, transport and transformation rates of pollutants in the soil, unsaturated and the saturated zones of the subsurface environment; (b) define the processes to be used in characterizing the soil and subsurface environment as a receptor of pollutants; (c) develop techniques for predicting the effect of pollutants on ground water, soil and indigenous organisms; and (d) define and demonstrate the applicability and limitations of using natural processes, indigenous to the soil and subsurface environment, for the protection of this resource.

Many contamination problems find their cause at or near the soil surface. Consequently, the physical and (bio-)chemical behavior of these contaminants in the shallow subsurface is of critical importance to the development of protection and remediation strategies. Mathematical models, representing our understanding of such behavior, provide tools useful in assessing the extent of pollution problems and evaluating means to prevent and remediate them. Increasingly, detailed understanding and subsequent modeling of the near-surface zone is crucial in designing effective remediation approaches. At many sites, this near-surface zone is only partially saturated with water, requiring specially designed mathematical models. This report focuses on models that might prove useful in simulating contaminant levels in such partially saturated systems.

The report is comprised of sections which overview considerations for modeling contaminant transport in the unsaturated system, procedures for identifying existing models, and criteria for the selection of models for application. The report includes appendixes which provide basic information on the authors, abstract, development and distribution institutions, purpose of development, and the availability of peer review information, documentation, verification/validation information, and literature citations for 92 unsaturated zone models.

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ABSTRACT

The present report contains the result of research and information processing activities supporting evaluation of the capabilities of various unsaturated zone flow and transport models in predicting the movement of hazardous chemicals through soils to ground water. It provides an overview of major types of models applicable to problems in the unsaturated zone of the subsurface. As chemical transport in soils is often driven by the movement of water, both flow and chemical transport models are included.

The review of models has been based on information gathered by the IGWMC through research and interviews on an on-going basis since 1978. To manage the rapidly growing amount of information, IGWMC maintains a descriptive model information system, MARS (Model Annotation Search and Retrieval System). Detailed information on the reviewed models is presented in a series of tables, preceded by an introduction on model classification, the principal characteristics of the described model types, and model selection issues.

BACKGROUND AND REPORT ORGANIZATION

EPA's R.S. Kerr Environmental Research Laboratory (RSKERL) Ada, Oklahoma and Environmental Research Laboratory (ERL) Athens, Georgia, on request of EPA/OERR, have initiated a project to evaluate how well various unsaturated zone flow and transport models can predict the movement of hazardous chemicals through soils to ground water. The project, referred to in this report as 'EPA-project', is divided in three components: 1) to identify available unsaturated/vadose zone models; 2) to collect and assimilate test data sets for model evaluation; and 3) to conduct sensitivity and evaluation tests.

The work assigned to the International Ground Water Modeling Center (IGWMC), referred to as 'IGWMC-project', addresses the issues identified as task 1 of the EPA-project: identifying and collecting information on available models, and cataloguing this information for use in the selection of models for evaluation.

The objective of the IGWMC-project was to develop a catalogue of available computer models, specifically designed to simulate the movement and fate of chemicals in the unsaturated/vadose zone. As the flow characteristics of the (liquid) water phase have an important influence on the movement of dissolved chemicals in the subsurface, the study has focussed on models or combinations of models that handle both flow and transport processes.

Additional analysis for this catalogue has focussed on the scenarios the models are designed to simulate through the incorporation of initial and boundary conditions and source and sink terms.

The catalogue, presented in Appendix 1 through Appendix 7, includes information on each model's author and institution of development, the code custodian, level of documentation, verification and peer review, and if it is proprietary or in the public domain. Model description comprises the model name, acronym, and an abstract describing its purpose, the processes it handles, the general mathematical method employed, and other major characteristics. Moreover, the catalogue includes information on media conditions, flow and fluid conditions, and type of boundary conditions handled by the model.

Finally, guidance is presented for the selection of models to be used in task 3 of the EPA-project, a detailed evaluation of selected models.

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1. MODELING IN THE UNSATURATED ZONE

1.1. INTRODUCTION

Until the early 1970's, modeling flow and transport through the unsaturated zone focused primarily on agricultural problems related to irrigation, drainage, and the application of fertilizers and pesticides. Since, such modeling has expanded to other type of problems due to increased public interest in solving ground-water pollution problems.

Pollution of subsurface water is typically described in terms of chemical composition. This chemical composition, often referred to as "water quality," is the result of natural processes and human intervention, either by introducing chemical compounds directly into the subsurface, or indirectly by modifying the effects of natural processes on the system. Although human intervention in the environment began many centuries ago, its significant effects on the quality of subsurface water are of recent origin, and in general are restricted to regions of significantly altered land use, as by urbanization, industrialization, mining, or agriculture. A major cause of widespread subsurface pollution is the introduction, purposely or accidentally, of solid and liquid wastes at the surface or in the near-surface soil and deep subsurface strata as a result of such land use. The introduced liquids and the leachate from solid waste are often highly mobile and chemically reactive, directly affecting subsurface water quality. It should be noted that in addition to the introduction of chemical compounds, ground-water pollution may result from the introduction into the natural system of hazardous biological compounds such as health-affecting bacteria and viruses.

Many contamination problems find their cause at or near the soil surface. Consequently, the physical and (bio-)chemical behavior of these contaminants in the shallow subsurface is of critical importance to the development of protection and remediation strategies. Mathematical models, representing our understanding of such behavior, provide tools useful in assessing the extent of pollution problems and evaluating means to prevent and remediate them.

In the context of this report, a major issue is determining the effectiveness of ground-water pollution remediation schemes. The performance of such schemes is generally reviewed in terms of rate of reduction in contaminant concentrations (either in ground water or in soils), the absolute time needed to reduce concentrations to regulatory limits, and the cost involved. For example, the Comprehensive Environmental Response, Compensation, and Liability Act of 1980 (CERCLA or Superfund), and the Superfund Amendments and Reauthorization Act of 1986 (SARA) require the establishment of soil remediation levels. Designing an effective remediation scheme requires site-specific knowledge of the influence of a variety of transport and fate processes on ground-water and soil contaminant levels. Mathematical models and their computer program representation provide a quantitative framework for assessment of the effectiveness of remediation designs taking into consideration the site-specific information obtained in the site characterization process.

Increasingly, detailed understanding and subsequent modeling of the near-surface zone is crucial in designing effective remediation approaches. At many sites, this near-surface zone is only partially saturated with water, requiring specially designed mathematical models. This report focuses on models that might prove useful in simulating contaminant levels in such partially saturated systems.

1.2. THE UNSATURATED ZONE

The subsurface hydrosphere is divided in various sub-systems or zones. Directly beneath the land surface is the zone of aeration, or *unsaturated zone*, which is partially filled with water (or non-aqueous phase liquids) and gases (mostly air). Other names used to identify the unsaturated zone, or regions where the pore space is not water-filled, are *vadose zone*, *variably saturated zone*, and *partially saturated zone*. The unsaturated zone thickness may vary widely in time and space. In wetlands this zone may be absent, while in arid areas the thickness of this zone can exceed 1000 m *[Bouwer, 1978]*. The root zone is that part of the unsaturated zone that supports plant growth. The root zone generally extends to a maximum depth of 2 m beneath the land surface *[Heath, 1983]*. Another term often used to describe the shallow subsurface is 'soil zone', defined as that part of the subsurface subject to soil forming processes. The soil zone includes the root zone and might extend to a depth of a few meters *[Hillel, 1982]*. The soil zone is a major interaction area between the subsurface hydrosphere, the surface hydrosphere, and the biospheric elements of terrestrial ecosystems on the other side.

The unsaturated zone is almost always underlain by rock layers that are fully saturated with liquids, primarily water. The volumetric water content of these saturated regions is equal to the porosity. This is the saturated zone, and the water in it is commonly referred to as *ground water*. Water in the unsaturated zone is commonly referred to as *soil water*.

At the boundary zone between the unsaturated and saturated zone, the attraction forces between water and rocks are balanced against the pull of gravity. As a result, the smaller pores are water-saturated while the larger pores contain both water and air. This boundary area between ground water and soil water is known as the capillary fringe. It is bounded at the bottom by the water table or the phreatic surface, the surface where the fluid pressure equals atmospheric pressure *[Bear 1979]*.

1.3. MODELING TRANSPORT AND FATE OF CONTAMINANTS IN THE UNSATURATED ZONE

Modeling contaminant behavior in the unsaturated zone is generally aimed to address such issues as *[NRC, 1990]*:

- Determining the arrival time of a contaminant at a certain depth; this requires a prediction of the travel time for the contaminant. Examples of depths of interest are the bottom of the

root zone, the bottom of the treatment zone of a hazardous waste land treatment system facility, or the water table.

- Predicting the amount of the surface-applied (or spilled) contaminant which might arrive at the depth of interest within a certain time (or mass flux passing this depth); this requires assessment of the transport, (temporary) retention, transformation and degradation (fate) of the contaminant.

- Predicting the concentration distribution or the contaminant mass flux in the unsaturated zone (in both the aqueous and solid phases) at a particular time, or their changes over time.

The latter purpose is of specific interest to this study as it relates to predicting the amount of hazardous constituents remaining in the soil following a soil remediation, or due to natural processes.

Contaminating chemicals may leave the soil zone by leaching downwards to the water table, by volatilization and escape to the atmosphere, by (bio-)chemical transformation or degradation, and by plant uptake *[Jury and Valentine, 1986]*. Leaching constitutes mass flow of a chemical constituent and is the product of water flux and dissolved chemical concentration. Mass flow is dependent on the amount of applied water, the water application intensity, the saturated hydraulic conductivity of the soil, the chemical concentration, the adsorption site density, and, indirectly, temperature *[Jury and Valentine, 1986]*. Soils provide a strong capacity for adsorbing chemicals and thus removing them from the amount of chemical subject to mass flux. This is due to the presence of electrically charged clay minerals and organic matter, and the large surface area of the minerals and humus. Hydrodynamic dispersion is a form of mass flow, the magnitude of which is subject to the scale over which the water flux is averaged. Volatilization of chemical vapor to the atmosphere takes place in the vapor phase of the soil and is controlled by chemical, soil, and atmospheric conditions. Volatilization is dependent on Henry's constant, chemical concentration, adsorption site density, temperature, water content, wind speed, and water evaporation. Other potentially important transport processes include vapor and liquid diffusion. Transformation and degradation processes determine the "fate" of the chemical of concern in the soil. The most important processes include chemical hydrolysis, biochemical transformations, and oxidation-reduction.

In classifying models generally applied to soil- and ground-water pollution problems, a distinction can be made between the transport of the contaminants from the point of their introduction into the subsurface (*i.e.*, contaminant source) to the location of concern (*e.g.*, point of exposure), and the (bio-) chemical transformations that may occur in the subsurface. A major transport mechanism results from the hydrodynamic behavior of contaminant carrying fluids or fluid phases in porous or fractured media. Models specifically simulating fluid flow are referred to as *flow* models. Models describing the movement of dissolved chemicals and their interaction with the soil or rock matrix in terms of concentrations and mass fluxes are often referred to as *contaminant transport models* or *solute transport models*. Furthermore,

models exist which are primarily concerned with (bio-)chemical transformations in the subsurface, and the resulting fate of contaminants. The latter type of models may be based on a simple mass balance approach for the chemical of concern lumping spatial variations in a single value for the parameters of interest (*e.g.*, SUMMERS model; *U.S. EPA, 1989*, pp. 28-29), or it may constitute a set of complex equations describing the (bio-)chemical reactions of interest including a reaction constant data base. To adequately simulate site-specific pollution problems and their remediation increasingly combinations of these three model types are employed (*e.g.*, *Yeh et al., 1993*).

The success of a given model depends on the accuracy and efficiency with which the physical and (bio-)chemical processes controlling the behavior of water and introduced non-aqueous liquids, and the chemical and biological species they transport, are simulated. The accuracy and efficiency of the simulation, in turn, depend heavily on the applicability of the assumptions and simplifications adopted in the model, the availability and accuracy of process information and site characterization data, and on subjective judgments made by the modeler and management.

As stated, flow models simulate the movement of one or more fluids in porous or fractured rock. One such fluid is water; the others, if present, can be air or vapors such as methane (in soil) or immiscible nonaqueous phase liquids (NAPLs; in both fully and partially saturated systems) such as certain solvents, sometimes having a density distinct from water (LNAPLs, DNAPLs). In the context of this report, only the flow of water (under unsaturated conditions) is considered. Most flow models are based on a mathematical formulation which considers the hydraulic system parameters as independent field information and hydraulic head, fluid pressure or water content and fluid flux as dependent variables. They are used to calculate: steady-state spatial distribution, changes in time in the spatial distribution, or the temporal distribution at a particular location of such variables as:

- hydraulic head, pressure head (or matric head), and suction head;
- saturation or moisture content;
- magnitude and direction of flow in terms of flow velocities or water mass fluxes;
- flowlines and travel times;
- position of infiltration fronts.

Inverse flow models simulate the flow field to calculate the spatial distribution of unknown system parameters using field or experimental observations on the state variables such as hydraulic head, fluid pressure, water content and fluid flux. Due to the complexity of the relationships between pressure head, saturation and hydraulic conductivity, there are no truly inverse models available for flow in partially saturated porous media.

The dominant parameter affecting flow and contaminant transport in the unsaturated zone is hydraulic conductivity. Accurate measurements of this parameter are difficult to make and very time-consuming. Therefor, theoretical methods have been developed to calculate the hydraulic conductivity from

more easily measured soil water retention data based on statistical pore-size distribution models *[van Genuchten et al., 1991]*. The resulting functional relationship between pressure head and volumetric water content (*i.e.*, soil water retention function) is presented in tabular form or as closed-form analytical solutions which contain functional parameters that are fitted to observed data. With the soil water retention function known the unsaturated hydraulic conductivity can be calculated using the model of Mualem *[1976]*. Models have been developed to fit mathematical functions to water retention with known hydraulic conductivity or to water retention and hydraulic conductivity simultaneously *[van Genuchten et al., 1991]*. These models may also be used to predict hydraulic conductivity for given soil retention data.

Solute transport models are used to predict movement or displacement, concentrations, and mass balance components of water-soluble constituents, and to calculate concentrations or radiological doses of soluble radionuclides *[van der Heijde et al., 1988]*. To do so, solute transport models incorporate various relevant physical and chemical processes. Flow is represented in the governing convective(-dispersive) equation by the flow velocity in the advective transport term. The velocities are also used for the calculation of the spreading by dispersion. If the velocity field is stationary, it may be either calculated once using an external flow program or read into the program as observed or interpreted data. If the velocity field (*i.e.*, spatial distribution of velocities in terms of direction and magnitude) is dependent on time and/or concentration, then calculation of velocities at each time step is required, either through an internal flow simulation module or an external flow model linked by means of input and output files. If a dissolved contaminant is present in relative high concentrations, changes in its distribution during the simulations might affect the flow behavior through changes in the fluid density. In that case, coupling of the flow and solute transport equations occur through an equation of state, resulting in a system of equations which needs to be solved simultaneously (*i.e.*, iteratively-sequentially *[Huyakorn and Pinder, 1983]*).

Generally, modeling the transformation and fate of chemical constituents is done in one of three possible ways *[van der Heijde et al., 1988]*: (1) incorporating simplified transformation or fate formulations in the equation describing solute transport; (2) formulating a mass-balance approach to (bio-)chemical transformation and fate; and (3) by coupling separate equations describing the (bio-)chemical processes with the advective-dispersive transport equation. Including transformation processes in solute transport models results in so-called nonconservative (*i.e.*, with respect to mass in solution) transport and fate models. The more complex of these nonconservative transport models may include advective and dispersive transport, molecular diffusion, adsorption (equilibrium and kinetics based), ion-exchange, radioactive decay, and (bio-)chemical decay.

In some cases, adequate simulation requires the assessment of the influence of temperature variations (and other physical properties) on flow, solute transport, transformation and fate. A few highly specialized multipurpose prediction models can handle combinations of heat and solute transport, and rock or soil matrix deformation. Generally, these models solve the system of equations in a coupled fashion to provide for analysis of complex interactions among the various physical, chemical, and biological processes involved.

In this report, only models simulating flow of water in the unsaturated zone and transport of dissolved chemicals in soil water will be discussed. Information on models simulating the flow of non-aqueous phase liquids (either in conjunction with water or as a separate contaminating fluid or contaminant transporting fluid) can be found in *van der Heijde et al., [1991]*, among others.

1.4. FLOW PROCESSES IN THE UNSATURATED ZONE

The mathematical model for flow of water in the subsurface is derived by applying principles of mass conservation (resulting in the continuity equation) and conservation of momentum (resulting in the equation of motion, *i.e.*, Darcy's law *[Bear, 1979]*). The most common governing equation for unsaturated flow is derived by combining the mass balance principle with Darcy's law, ignoring compressibility effects of matrix, fluid, and air. The resulting equation, known as Richards' equation, is the basis for many unsaturated zone models *[Bear, 1979; DeJong, 1981; El-Kadi, 1983; Jury et al., 1991]*. The dependence of the hydraulic properties of partially porous media on the hydraulic head or degree of saturation makes the Richard's equation nonlinear. The degree of nonlinearity depends on the nature of the relationship between hydraulic conductivity and hydraulic head or saturation, which is often highly nonlinear *[Huyakorn and Pinder, 1983]*.

In general, the state variable for saturated flow is piezometric head or fluid pressure. The flow equation for the unsaturated zone may be expressed in one of two types of state variables, or a combination: 1) fluid pressure, hydraulic head, pressure head (*i.e.*, matric head), or suction (*i.e.*, negative pressure head); and 2) moisture content or saturation. Fluid pressure is related to moisture content through the soil water characteristic curve or soil moisture retention curve. Often, different curves exist for when the moisture content in a particular soil increases (*i.e.*, wetting curve) and decreases (*i.e.*, drying curve), a phenomenon called hysteresis. If hysteresis is important the saturation formulation of the Richard's equation might be preferable as saturation is less sensitive to hysteresis *[Hillel, 1982]*.

In order to solve the transient flow equation, both initial and boundary conditions are necessary. Initial conditions consist of given values for the dependent variable throughout the model domain representing the system's status at the beginning of the simulation. For most models, inclusion of initial conditions is only needed when transient simulations are performed. Boundary conditions may be any of three types: specified value for the dependent variable (Dirichlet or first type), specified value for the derivative of the dependent variable perpendicular to the boundary (Neumann type or second type), and mixed (Cauchy or third type) conditions. Boundary conditions are specified on the periphery of the modeled domain, either at the border of the modeled area or at internal boundary locations where responses are fixed (*e.g.*, fluxes in or out of the system through subsurface irrigation pipes or drains, respectively).

The mathematical formulation and solution of the flow problem in the unsaturated zone require describing the hydraulic properties of soil, preferably in functional form. Hysteresis usually influences these functions. However, simulation under hysteresis is difficult due to the existence of an infinite number of

drying and wetting curves, depending on the wetting-drying history of the soil. Several examples of algebraic equations to represent the soil water characteristic curves with no hysteresis are available *[Brooks and Corey, 1966; Gardner [1958] as used by Haverkamp et al., 1977; van Genuchten, 1980].*

Another complication is the existence of structural voids such as cracks, root holes and animal channels, often called macropores or macrochannels *[Jury et al., 1991]*. As these macrochannels might provide important conduits for rapid downward migration of contaminants, for certain field conditions models might be needed that are able to represent the transport through such macro features as well as through the porous media.

1.5. BOUNDARY CONDITIONS FOR UNSATURATED FLOW

Solution of the partial-differential equations for unsaturated flow requires the specification of initial and boundary conditions in terms of the relevant state variable *[Bear, 1979]*. In many cases it is important to specify if a drying or wetting process is taking place along the boundary due to hysteresis in the soil water characteristic curve. The following boundary conditions may be encountered in the unsaturated zone *[Bear, 1979; Bear and Verruijt, 1987]*:

- *Prescribed water content* (or piezometric head, pressure, or suction) at all points of the boundary. This is the Dirichlet boundary condition. For example, such a condition is present when ponding occurs at the soil surface (under practical circumstances, it might be more difficult to define this condition for the other state variables). At the phreatic surface, generally considered the lower boundary of the unsaturated zone, the boundary condition is that of zero fluid pressure.

- *Prescribed flux of water.* This occurs when water reaches the soil surface at a known rate (*e.g.*, rainfall and sprinkler irrigation) or when the boundary is impervious to water (*i.e.*, zero flux). Dependent on the presence or absence of a gravity term in the quantification of the boundary condition, prescribed flux is either a boundary condition of the third or second kind, respectively.

Under certain circumstances, the boundary condition at the soil surface may change from a prescribed flux to a prescribed water content. This is the case when the accretion rate at the surface exceeds the infiltration capacity of the soil surface. Another boundary flux is evaporation. This boundary flux is dependent on antecedent soil moisture conditions, and soil moisture related limitations on boundary flux might develop over time, requiring special measures in the implementation of such conditions in models. Finally, a third-type boundary condition exists when the soil is covered by a water body, separated from the soil by a semi-pervious layer (*e.g.*, the bottom of a pond).

1.6. MODELING SOURCES OF SUBSURFACE POLLUTION

When using models to analyze soil contamination problems, the contamination source must be adequately described in terms of spatial, chemical, and physical characteristics and temporal behavior. The spatial definition of the source includes location, depth, and areal extent. Model representation of the source depends on spatial and temporal characteristics and on the scale of modeling. Typical model representations of pollution sources include a point source for one-, two- and three-dimensional models, and a line source, a distributed source of limited extent, and a non-point source of unlimited extent for two- and three-dimensional models.

The source can be located at the boundary or within the system for which the model is developed, dependent on the dimensionality of the model among others. Mathematically, contaminant sources can be simulated as a boundary condition, or through specific, closely connected source terms in the governing flow and transport equations. Typically, if a source is represented as boundary condition, a third-type transport boundary condition is chosen.

To represent a source accurately, the location of the source with respect to the model domain needs to be defined. When the source lies outside or at the edge of the domain it is considered a boundary source, represented by either a formal boundary condition or by a boundary source/sink term (dependent on the mathematical formulation of the model). If the modeled domain is the unsaturated zone of the subsurface, such a source might be an impoundment, surface spill, or waste pile. When the source lies within the model domain, it is considered an internal source which may only be represented by an internal source/sink function. Often internal sources are present as a secondary source resulting from temporary attenuation of contaminants released by a surface source followed by delayed release ("bleeding" *[NRC, 1990]*) of the contaminant to the water table. If the source is a boundary source represented by a boundary condition, the model selected needs to facilitate the proper boundary condition (specified concentration, specified mass flux, or concentration-gradient dependent mass flux).

The extent of the simulated plume is influenced by the choice of the source's spatial dimensions. The areal extent of the source in relation to the modeling scale determines the spatial character of the source in the model. In some cases a non-point pollution source for a local scale model is considered a point pollution source for modeling at a regional scale (e.g., septic tanks, landfills, feedlots).

Another source characteristic important to the modeling process is source history, or expected behavior in time. The source can be continuous in time, either fluctuating or constant in strength (*e.g.*, landfills, impoundments, feedlots), or in the form of a pulse or series of individual, non-overlapping pulses (*e.g.*, spills, leaching of agro-chemicals during or after a storm).

It should be noted that to correctly represent the source, often, both flow and transport boundary conditions or flow and transport source terms are involved.

1.7. ANALYTICAL AND NUMERICAL SOLUTIONS

Most mathematical models for the simulation of flow and solute transport in the unsaturated zone are distributed-parameter models, either deterministic or stochastic *[van der Heijde et al., 1988]*. Their mathematical framework consists of one or more partial differential equations describing the flow and/or transport and fate processes, as well as initial and boundary conditions and solution algorithms. Some of these models assume that the processes active in the system are stochastic in nature or, at least, that the process variables may be described by probability distributions. In such stochastic models system responses are characterized by statistical distributions estimated by solving a deterministic governing equation.

The governing equations for flow and transport in the unsaturated zone are usually solved either analytically or numerically. Analytical models contain a closed-form or analytical solution of the field equations subject to specified initial and boundary conditions. To obtain these analytical solutions, simplifying assumptions have to be made regarding the nature of the soil-water-solute system, geometry, and external stresses, often limiting their application potential. Because of the complex nature of single and multi-phase flow in the unsaturated zone and the resulting nonlinearity of the governing equation(s) very few analytical flow solutions have been published *[Bear, 1979]*. With respect to transport and fate the situation is somewhat different. Many one-, two-, and three-dimensional analytical solutions for the classical convection-dispersion equation exist, often requiring a uniform flow field. Some of these solutions, specifically one-dimensional solutions, can be used in the unsaturated zone assuming a uniform vertical soil water flux.

In semi-analytical models, complex analytical solutions are approximated, often using numerical techniques. In the case of unsaturated flow, semi-analytical solutions may be derived by using analytical expressions for the relationships between the dependent variables and the hydraulic parameters and involving numerical integration *[Bear, 1979]*. Models based on a closed-form solution for either the space or time domain, and which contain additional numerical approximations for the other domain, are also considered semi-analytical models. Various quasi-analytical techniques and approximate (analytical) equations have been developed for simulating infiltration of water in soils *[El-Kadi, 1983]*. The same holds true for the one-dimensional transport of solutes *[van Genuchten and Alves, 1982]*.

In numerical models, a discrete solution is obtained in both the space and time domains by using numerical approximations of the governing partial differential equation. As a result of these approximations the conservation of mass and accuracy in the prediction variable are not always assured (because of truncation and round-off errors) and thus needs to be verified for each application. Spatial and temporal resolution in applying such models is user-defined. If the governing equations are nonlinear, as is the case in simulating flow in the unsaturated zone, linearization often precedes the matrix solution *[Remson et al., 1971; Huyakorn and Pinder, 1983]*. Usually, solution of nonlinear equations is achieved employing nonlinear

matrix methods such as the Picard, Newton-Raphson, and Chord-Slope methods *[Huyakorn and Pinder, 1983]*.

The numerical solution techniques used for approximating the spatial components of the governing flow equations in the unsaturated zone are primarily the finite-difference methods (FD), the integral finite-difference methods (IFDM), and the Galerkin finite-element method (FE). In most cases, time is approximated by finite difference techniques resulting in an explicit, (weighted) implicit or fully implicit solution scheme. A finite-difference solution is obtained by approximating the derivatives of the governing equation. In the finite-element approach an integral equation is formulated first, followed by the numerical evaluation of the integrals over the discretized flow or transport domain. The formulation of the solution in each approach results in a set of algebraic equations which are then solved using direct or iterative matrix methods. Specific schemes may be required for the constitutive relationships, specifically in the presence of hysteresis.

There are many numerical considerations in selecting a model for simulation of a particular soil-water-solute system. Simulating flow in relative wet soils (*e.g.*, nearly saturated conditions and ponding) requires expression of the Richard's equation in terms of hydraulic head, matric head or suction head, especially when parts of the modeled soil system become fully saturated. However, application of this form of the Richard's equation causes significant convergence problems when simulating an infiltration front in extremely dry soil conditions; in the latter case formulation of Richard's equation should be based on saturation or mixed pressure-saturation *[Huyakorn and Pinder, 1983; Celia et al., 1990]*. An advantage of the mixed form is that it allows the transition from unsaturated to saturated conditions while maintaining numerical mass conservation *Celia et al., 1990)*. Also, significant mass balance problems might occur when site-specific conditions result in highly nonlinear model relationships *[Celia et al., 1990]*.

Other issues that should be addressed in selecting a model for simulating flow in the unsaturated zone are the possible need for double precision versus single precision variables, the time-stepping approach incorporated, the definition used for intercell conductance (*e.g.*, harmonic mean versus geometric mean), and, if present, the way steady-state simulation is achieved (most models do not provide steady-state flow solutions). Some of the problems one may encounter with specific models (or modeling techniques) include code limitations on gridding flexibility, numerical problems in zones with high-contrast soil or rock properties, and inaccuracy and instability in areas where the flow field changes significantly in magnitude and direction. In some cases, avoiding inaccuracy and instability problems require very small spatial and temporal increments, making multi-dimensional simulations expensive or even unfeasible. Sometimes, an adaptive time-stepping scheme is implemented in the computer program to optimize time step requirements.

Typical numerical techniques encountered in solving the convective-dispersive solute transport equation in the unsaturated zone are comparable to those employed in simulating solute transport in the saturated zone and include various finite-difference methods, the integral finite-difference method, various Galerkin finite-element formulations, and variants of the method of characteristics *[Yeh et al., 1993]*. As with

flow, time is generally approximated by finite difference techniques resulting in an explicit, (weighted) implicit or fully implicit solution scheme.

Typical problems found in applying traditional finite difference and finite element techniques to simulate contaminant transport in both the saturated and unsaturated zones include numerical dispersion and oscillations. Numerical dispersion is referred to when the actual physical dispersion mechanism of the contaminant transport cannot be distinguished from the front-smearing effects of the computational scheme *[Huyakorn and Pinder, 1983]*. For the finite-difference method, this problem can be reduced by using the central difference approximation. Spatial concentrations oscillations (and related overshoot and undershoot) may occur near a sharp concentration front in an advection-dominated transport system. Remedies for these problems are found to some extent in the reduction of grid increments or time step size, or by using upstream weighing for spatial derivatives. The use of weighted differences (combined upstream and central differences) or the selection of other methods (*e.g.*, the method of characteristics, and the Laplace transform Galerkin method) significantly reduces the occurrence of these numerical problems.

1.8. DATA REQUIREMENTS

The number and type of parameters required for modeling flow and transport processes in soils depend on the type of model chosen. These parameters can be divided in control parameters (controlling the operation of the computer code), discretization data (grid and time stepping), and material parameters. The material parameters can be grouped in six sets *[Jury and Valentine, 1986]*: static soil properties, water transport and retention functions, basic chemical properties, time-dependent parameters, soil adsorption parameters, and tortuosity functions. Table 1 lists many of the relevant material model parameters. To illustrate the variety of input requirements for different types of models, appendix 8 lists the input requirements of four selected unsaturated zone models: RITZ, FLAME/FLASH, MULTIMED, and VS2D/T.

Table 1. Selected Material Parameters for Flow and Transport Parameters in Soils (After *Jury and Valentine, 1986*)

Static Soil Properties
- porosity
- bulk density
- particle size
- specific surface area
- organic carbon content
- cation exchange capacity
- pH
- soil temperature

Flow and Transport Variables and Properties
- saturated hydraulic conductivity
- saturated water content
- matric head-water content function
- hydraulic conductivity function
- dispersion coefficient or dispersivity

Basic Chemical Properties
- molecular weight
- vapor pressure
- water solubility
- Henry's constant
- vapor diffusion coefficient in air
- liquid diffusion coefficient in water
- octanol-water or oil-water partition coefficient
- half-life or decay rate of compound
- hydrolysis rate(s)

Contaminant Source Characteristics
- solute concentration of source
- solute flux of source
- source decay rate

Time dependent parameters
- water content
- water flux
- infiltration rate
- evaporation rate
- solute concentration
- solute flux
- solute velocity
- air entry pressure head
- volatilization flux

Soil Adsorption Parameters
- distribution coefficient
- isotherm parameters
- organic carbon partition coefficient

Tortuosity Functions
- vapor diffusion tortuosity
- liquid diffusion tortuosity

2. IDENTIFICATION OF MODELS

2.1. PROCEDURES

To identify existing models for simulation of flow and contaminant transport in the unsaturated subsurface, a database search and literature review has been conducted. Initially, the database search was focussed on the MARS model annotation database of the IGWMC, which as of May 1992 contains about 650 descriptions of soil- and ground-water simulation models. Information for the literature review has been obtained from various sources, including the IGWMC literature collection of more than 3000 titles and about 20 serials, and through interlibrary loan. Additional information was received from the U.S. EPA Center for Subsurface Modeling Support (CSMoS) located at RSKERL, Ada, Oklahoma.

New information on characterized models as well as information on new models have been added to the MARS database. This updated database has been used in an early stage of the project to provide the EPA-project team with an interim overview of identified models. The final report contains descriptions of models which have been identified after the submittal of the interim report, or which have been recently released.

After reviewing the model's documentation and other pertinent literature obtained, contact has been sought with model authors and code custodians to obtain additional information when necessary.

In the process of collecting information for the catalogue, parameter needs and other input requirements for selected models have been assessed (Appendix 8). An evaluation of eight flow and transport models applicable to contaminated soil cleanup provided additional direction for this assessment *[C. Pratt, State of Washington, Dept. of Ecology, 1991, personal communication]*. Selected models have been described with respect to the way they handle source characterization (in both time and space), dimensionality, boundary conditions, and transport and fate processes. Where appropriate, this information has been added to the abstract or to the remarks for the individual models. Furthermore, this information has been used to update the MARS check list of code characteristics (Appendix 9).

2.2. MODEL INFORMATION SYSTEM

To be able to select a computer code appropriate for the site- or problem-specific analysis to be performed, ground-water modelers need to have an overview of available computer codes and their characteristics. Since its establishment in 1978, IGWMC has been collecting, analyzing, and disseminating information on ground-water models, first from the Holcomb Research Institute at Butler University, Indianapolis, Indiana, and since mid-1991 from the Colorado School of Mines, Golden, Colorado. IGWMC has developed a systematic approach to classify, evaluate and manage descriptive information regarding ground-water modeling codes for the purpose of model selection. To manage the continuously growing

amount of information, IGWMC maintains a descriptive model information system, MARS (Model Annotation Search and Retrieval System) *[van der Heijde and Williams, 1989]*.

Each model is described in an uniform way by a set of annotations describing its purpose, major hydrological, mathematical and operational characteristics, input requirements, simulative capabilities, level of documentation, availability, and applicability. A complete model annotation includes comments made by the model author and IGWMC staff concerning development, testing, quality assurance and use, as well references of studies using the model and references that are part of the documentation or considered pertinent to the model. The checklist used by the IGWMC to characterize ground-water models is given in Appendix 9.

Based on the analysis of the needs for information on ground-water models, five types of potential use have been identified:

- application to field problems in support of policy-making and resource management decisions;
- analyzing field and laboratory experiments as part of a research program;
- as basis for new model formulations and software development;
- in education regarding modeling principles and training in the use of models; and
- verification of and comparison with other models.

The content and structure of the database is thus a consequence of a primary objective: identification of models for any of the above uses.

The IGWMC staff continuously collects and analyzes information on models related to subsurface flow and transport phenomena. The initial information may come from open literature or from presentations and discussions at conferences, workshops, and other meetings, or obtained directly from researchers.

Once a model of interest is located, additional information is collected from the research team that developed the model, and from pertinent literature to enable the IGWMC staff to include the model in the MARS database. In selecting a model for inclusion in the referral database, special attention is given to the importance of the model with respect to the kind of questions raised in model-based problem solving, and to the development status of the model (*e.g.*, research instrument or deliverable versus a generally applicable, well-tested and documented routine tool).

To assure consistency in the evaluation of the model information and data entered in the referral database, a standardized form (MARS data entry form) has been designed. A complete data set annotation includes comments made by the original development team and the IGWMC staff, as well as bibliographic references regarding development, theoretical foundation, updating, and use. After detailed evaluation of the model documentation by the IGWMC staff, data is entered into MARS. Once all the information describing a model is entered in the referral database, the information is checked for completeness and data entry errors.

In order to fulfill the growing and changing information needs of users, comprehensive and flexible procedures for maintaining, updating, and expanding the databases have been adopted. Every few years the database structure (programs and record structure) and contents are reviewed and revised.

3. MODEL SELECTION

3.1. SELECTION PROCESS

Based on the objectives of a project and the characteristics of the soil system involved, the need for and complexity level of mathematical simulation must be determined. If a model is needed, careful code selection is critical in ensuring an optimal trade-off between effort and result. The result is generally expressed as the expected effectiveness of the modeling effort in terms of forecast accuracy. The effort is ultimately represented by the costs. Such costs should not be considered independently from those of field data acquisition. For proper assessment of modeling cost, such measures as choice between the development of a new code or the acquisition of an existing code; the implementation, maintenance, and updating of the code; and the development and maintenance of databases and their interfacing with the simulation codes, need to be considered.

As code selection is in essence matching a detailed description of the modeling needs with well-defined characteristics of existing models, selecting an appropriate model requires analysis of both the modeling needs and the characteristics of existing models. Major elements in evaluating modeling needs are:

(1) formulation of the management objective to be addressed and the level of analysis sought (based among others on the sensitivity of the project for incorrect or imprecise answers or risk involved);

(2) knowledge of the physical system under study; and

(3) analysis of the constraints in human and material resources available for the study.

To select models efficiently, management-oriented criteria need to be developed for evaluating and accepting models. Such a set of scientific and technical criteria should include:

- Trade-offs between costs of running a model (including data acquisition for the required level of analysis) and accuracy;
- A profile of model user and a definition of required user-friendliness;
- Accessibility in terms of effort, cost, and restrictions; and
- Acceptable temporal and spatial scale and level of aggregation.

If different problems must be solved, more than one model might be needed, or a model might be used in more than one capacity. In such cases, the model requirements for each problem posed have to be clearly defined at the outset of the selection process. To a certain extent this is also true for modeling the same system in different stages of the project. Often a model is selected in an early stage of a project to assist in problem scoping and system conceptualization. Limitations in time and resources and in data availability might initially force the selection of a "simple" model. Growing understanding of the system and increasing data availability might lead to a need for a succession of models of increasing complexity. In such cases, flexibility of the candidate model or the availability of a set of integrated models of different levels of sophistication might become an important selection criterion.

The major model-oriented criteria in model selection are:

(1) that the model is suitable for the intended use;

(2) that the model is reliable; and

(3) that the model can be applied efficiently.

The reliability of a model is defined by the level of quality assurance applied during development, verification and field testing. A model's efficiency is determined by the availability of its code and documentation and its usability, portability, modifiability, and economy with respect to human and computer resources required.

As model credibility is a major problem in model use, special attention should be given in the selection process to ensure the use of qualified models that have undergone adequate review and testing according to standardized review and testing procedures *[van der Heijde and Elnaway, 1992]*.

Finally, acceptance of a model for decision-support use should be based on technical and scientific soundness, user-friendliness, and legal and administrative considerations.

A model's ability to meet management's information needs and its efficiency in obtaining the answers sought, are important selection criteria. In evaluating a model's applicability to a problem, a good description of operating characteristics should be accessible. Elements of such a description are given in Appendix 9.

Although adequate models are available for analysis of single phase flow problems in soils, modeling contaminant transport and fate in soils is significantly more problematic. Consequently, the use of models for water quality assessments in soils is generally restricted to conceptual analysis of pollution problems, to feasibility studies in design and remedial action strategies, and to data acquisition guidance. It should be noted that considering the uncertainties associated with the parameters of soil systems *[Jury, 1986]*, it

is more feasible to determine the probabilities of the time of arrival of a pollution front than the probabilities of concentration distributions in space or time.

A perfect match rarely exists between desired characteristics and those of available models. Model selection is partly quantitative and partly qualitative. Many of the selection criteria are subjective or weakly justified often because there are insufficient data in the selection stage of the project to establish the importance of certain characteristics of the system to be modeled. If a match is hard to obtain, reassessment of these criteria and their relative weight in the selection process is necessary. Hence, model selection is very much an iterative process.

In selecting models for the simulation of transport and fate of contaminants in the unsaturated zone, all relevant physical and (bio-)chemical processes active in the shallow subsurface need to be considered, as well as the planned measures to abate the contamination. Few models exist that are so general and all-encompassing in their design that they can be used for every situation encountered in the field. In selecting models for this review, it was recognized that a combination of models rather than a single model might be necessary to achieve the objectives of the user. As the flow regime present in the subsurface has a major influence on the transport of chemicals, ample attention is given to models that simulate water flow in the unsaturated zone (Appendix 2) and programs that assist in the determination of hydraulic parameters from laboratory and field studies (Appendix 7). Furthermore, the report presents models which simulate water flow and solute transport and fate, either in coupled or uncoupled fashion (Appendix 3), and models which simulate only solute transport and fate requiring a known flow field (Appendix 4). Finally, models are listed which either handle flow and heat transport (Appendix 5), or combined flow, solute transport and heat transport to facilitate the incorporation of the effects of temperature distributions and variations in time on flow, transport and fate (Appendix 6).

The report does not discuss models which are based on approximate infiltration equations as these equations are considered less relevant with respect to advective transport of contaminants. A discussion of such models can be found in El-Kadi *[1983]*. Also, the report does not discuss models which handle multi-phase flow (*i.e.*, water and non-aqueous phase liquids). More information on multi-phase flow (and transport) models can be found in Abriola *[1988]* and El-Kadi *et al. [1991]*. The report lists a limited number of nitrogen/phosphorus transport models. Additional information on such models can be found in Frissel and van Veen *[1981]*, Iskander *[1981]*, Tanji *[1982]*, De Willegen *et al. [1988]*, and Vachaud *et al. [1988]*.

3.2. RELIABILITY, USABILITY, AND OTHER CONSIDERATIONS

A model's efficiency is determined by the availability of an operational computer code and complete, well-organized documentation, access to user support, and by its usability, portability, modifiability, reliability, and economy. A brief discussion of some of these criteria is given below.

Availability

A model is defined as available if the program code associated with it can be obtained either as a compilable source code or as an already compiled run-time version. Available ground-water modeling software is either public domain and proprietary. In the United States, most models developed by federal or state agencies or by universities through funding from such agencies are available without restrictions in use and distribution, and are therefore considered to be in the public domain. The situation in other countries is often different, with most software having a proprietary status, even if developed with government support, or its status is not well-defined. In these cases, the computer code can be obtained or accessed under certain restrictions of use, duplication, and distribution.

Models developed by consultants and private industry are often proprietary. This may also be true of software developed by some universities and private research institutions. Proprietary codes are in general protected by copyright law. Although the source codes of some models have appeared in publications such as textbooks, and are available on tape or diskette from the publisher, their use and distribution might be restricted by the publication's copyright.

Further restrictions occur when a code includes proprietary third-party software, such as mathematical or graphic subroutines. For public domain codes, such routines are often external and their presence on the host-computer is required to run the program successfully.

Between public domain and proprietary software is a grey area of so-called freeware or user-supported software. Freeware can be copied and distributed freely, but users are encouraged to support this type of software development with a voluntary contribution.

It should be noted that for some codes developed with public funding, distribution restrictions are in force, as might be the case if the software is exported, or when an extensive maintenance and support facility has been created. In the latter case, restrictions are in force to avoid use of non-quality-assured versions, to prevent non-endorsed modification of source code, and to facilitate efficient code update support to a controlled user group.

The major advantage of public domain software is the absence of restrictions regarding its use, distribution, and modification. However, many public domain models are not as well supported and maintained as certain commercially distributed proprietary models. Because no mechanism exists to certify modeling software and their modifications, quality assurance of public domain software is a major problem, especially if more than one version exists.

Reliability

Reliability is the capability of a code to: 1) obtain computational results in a mathematically straightforward fashion (*i.e.*, converging); 2) reproduce consistent results (*i.e.*, obtain the same results when executed repeatedly in the same computational environment with the same data set); 3) produce results with an accuracy determined by resource utilization (*e.g.*, grid scale and time-step size); and 4) produce correct results (*i.e.*, provide or converge to the correct answer). The reliability of codes should be established by applying a widely accepted review and testing procedure. Such testing is aimed at removing programming errors, testing embedded algorithms, and evaluating the operational characteristics of the code through its execution on carefully selected example data sets (either based on analytical solutions, hypothetical problems, or existing field or laboratory experiments). It is important to distinguish between code testing and model testing. Code testing is limited to establishing the correctness of the computer code with respect to the criteria and requirements for which it is designed and to establish the accuracy and efficiency of the code within the range of anticipated field conditions. Model testing is more inclusive (and often more eluding) than code testing, as it represents the final step in determining the validity of the quantitative relationships derived for the real-world prototype system the model is designed to simulate *[van der Heijde et al., 1988]*.

A major issue in model use is credibility. A model's credibility is based on its proven reliability and the extent of its use. Model users and managers often have the greatest confidence in those models most frequently applied. This notion is reinforced if successful applications are peer-reviewed and published. As reliability of a program is related to the localized or terminal failures that can occur because of software errors, it is assumed that most such errors originally present in a widely used program have been detected and corrected. Yet no program is without programming errors, even after a long history of use and updating. Some errors will never be detected and do not or only slightly influence the program's utility. Other errors show up only under exceptional circumstances. Decisions based on the outcome of simulations will be viable only if the models have undergone adequate review and testing. However, relying too much on comprehensive verification, extensive field testing (if present), or frequency of model application may exclude certain well-designed and documented models, even those most efficient for solving the problem at hand.

Extent of Model Use

A model used by a large number of people demonstrates significant user confidence. Extensive use often reflects the model's applicability to different types of ground-water systems and to various management questions. It might also imply that the model is relatively easy to use. Finally, if a model has a large user base, many opportunities exist to discuss particular applications with knowledgeable colleagues.

Efficiency

Model efficiency is defined as the ratio between the accuracy obtained and the level of effort, in terms of human and computer resources, to reach that accuracy. A model's efficiency can be established by performance testing of the computer code and comparing computational results with benchmarks representative for the range of application environments anticipated (in terms of system schematization, parameter values, boundary conditions, and system stresses, among others). Establishing actual criteria such as CPU time, RAM requirements, I/O time, mass storage requirements, and set-up time measurements are needed. Reliability and efficiency are the main foci of performance testing of models.

User Support

If a model user has decided to apply a particular model, technical problems may be encountered in running the model code on the available computer system. Such a difficulty may result from (1) compatibility problems between the computer on which the model was developed and the model user's computer; (2) coding errors in the original model; and (3) user errors in data input and model operation.

User-related errors can be reduced by becoming more familiar with the model. Here the user benefits from good documentation. If, after careful selection of the model, problems in implementation or execution of the model occur and the documentation does not provide a solution, the user needs help from someone who knows the code. Such assistance, called model support, cannot replace the need for proper training in model use; requests for support from model developers may reach such extensive proportions that model support becomes a consulting service or an on-the-job training activity. This potential is generally recognized by model developers, but not always by model users.

Usability

Various problems can be encountered when a simulation code is implemented on the user's computer system. Such difficulties may arise from hardware incompatibilities or coding of user errors in code installation, data input, or program execution. Programs that facilitate rapid understanding, knowledge of their operational characteristics, and are easy to use are called user-friendly and defined by usability. In such programs, emphasis is generally placed on extensive, well-edited documentation, easy input preparation and execution, and well-structured, informative output. Adequate code support and maintenance also enhance the code's usability.

Portability

Programs that can be easily transferred from one computer environment to another are called portable. To evaluate a program's portability both software and hardware dependency need to be considered.

Modifiability

In the course of a computer program's useful life, the user's experiences and changing management requirements often lead to changes in functional specifications for the software. In addition, scientific developments, changing computing environments, and the persistence of errors make it necessary to modify the program. If software is to be used over a period of time, it must be designed so that it can be continually modified to keep pace with such events. A difficult to modify code is called fragile and lacks maintainability. Such difficulties may arise from global, program-wide implications of local changes.
If the program needs to be altered to run in a new computer environment, its modifiability is important. Modifiability is enhanced by working with a well-maintained program language environment which adheres to established language standards; by using structured, object-oriented programming techniques and modular program designs; and by the presence of programmer-oriented documentation including program flow charts, definition of key variables, discussion of data transfer between the subroutines and functions, description of purpose and structure individual subroutines and functions, and extensive internal documentation listing the purpose of individual code segments.

4. CONCLUDING STATEMENT

This report provides a catalogue of close to 100 flow and transport models which may be used for the simulation of flow and transport processes in the unsaturated zone, among others to determine the effectiveness of soil remediation schemes. The models considered range from simple mass balance calculations to sophisticated, multi-dimensional numerical simulators. This report does not pretend be complete in its listing of appropriate models. Almost every week, the International Ground Water modeling Center is informed of new computer codes addressing some aspect of fluid flow and contaminant transport in the subsurface. Moreover, many codes have been developed primarily for research purposes and are not very accessible. Also, there are many simple models based on mass balance evaluation or analytical solution of highly simplified systems not presented in this catalogue. An effort has been made to select those 'simple' models which are either known for their use in an regulatory or enforcement mode, or which are considered representative for a certain type of models. This report does not discuss multi-fluid flow and associated transport of contaminants since a considerable amount of research is currently focussed on understanding and mathematically describing the physics and chemistry of these systems.

There are six categories of models listed, including models for single-fluid flow, coupled and uncoupled flow and solute and/or heat transport, and solute transport for given pressure head distribution. Finally, models are listed which provide soil parameters from column experiments on soil samples.

Although adequate models are available for analysis of single phase flow problems in soils, modeling contaminant transport and fate in soils is significantly more problematic. Consequently, the use of models for water quality assessments in soils is generally restricted to conceptual analysis of pollution problems, to feasibility studies in design and remedial action strategies, and to data acquisition guidance. Considering the uncertainties associated with the parameters of soil systems, it is more feasible to determine the probabilities of the time of arrival of a pollution front than the probabilities of concentration distributions in space or time.

In compiling the information for the catalogue, some relevant issues have arisen. In many cases, model documentation is insufficient to determine the actual implementation of boundary conditions in the code, or the required detail in discretization in the spatial and temporal domains. Running a model code, using test problems different than the example problems given in the documentation, might reveal specific model characteristics (and "tricks" to handle them), accuracy, stability, or execution problems. Furthermore, there are few models which handle the complete spectrum of unsaturated zone flow and solute transport conditions encountered in the field. For example, many models encounter problems in simulating steep infiltration or concentration fronts.

A systematic performance testing procedure for unsaturated zone models should be developed to address these issues by incorporating test problems and scenarios which document the range of geometries, parameter values and boundary conditions which the model can handle adequately, and which

will reveal situations where the model's behavior is suspect or unsatisfactory. This type of testing should be performed parallel to the kind of testing which uses independently observed systems such as well-documented, carefully executed field and laboratory experiments.

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van Genuchten, M.T. 1980. A Closed-Form Equation for Predicting the Hydraulic Conductivity of Unsaturated Soils. Soil Sci. Soc. of Am. Journ.. Vol. 44, pp. 892-898.

van Genuchten, M.Th., and W.J. Alves. 1982. Analytical Solutions of the One-Dimensional Convective-Dispersive Solute Transport Equation. Techn. Bull. 1661, U.S. Dept. of Agriculture, Riverside, Calif.

van Genuchten, M.Th., F.J. Leij, and S.R. Yates. 1991. The RETC Code for Quantifying the Hydraulic Functions of Unsaturated Soils. EPA/600/2-91/065, U.S. Environmental Protection Agency, R.S. Kerr Environmental Research Lab., Ada, Oklahoma.

Yeh, T.-C., R. Srivastava, A. Guzman, and T. Harter. 1993. A Numerical Model for Water Flow and Chemical Transport in Variably Saturated Porous Media. Ground Water, Vol. 31(4), pp. 634-644.

Appendix 1: Cross-reference Table for Unsaturated Zone Models

MODEL NAME	FIRST AUTHOR	IGWMC KEY	PAGE
3DFEMWATER/3DLEWASTE	Yeh, G.T.	3377	A-3-5
BIOSOL	Baek, N.H.	5021	A-3-18
CADIL/AGTEHM	Emerson, C.J	4290	A-3-8
CHAIN	van Genuchten, M.A.	6225	A-4-3
CHEMFLO	Nofziger, D.L.	6712	A-3-22
CHEMRANK	Nofziger, D.L.	6640	A-3-17
CMIS	Nofziger, D.L.	6710	A-3-19
CMLS	Nofziger D.L.	6711	A-3-20
CREAMS	Knisel, W.G.	3540	A-3-6
CTSPAC	Lindstrom, F.T.	5031	A-6-4
DISPEQ/DISPER/PISTON	Fluhler, H.	3450/ 3451	A-3-5
DRAINMOD	Skaggs, R.W.	1950	A-3-2
FEMTRAN	Martinez, M.J.	4350	A-4-1
FEMWASTE/FECWASTE	Yeh, G.T.	3371	A-4-1
FEMWATER/FECWATER	Yeh, G.T.	3370	A-2-10
FLAME	Baca, R.G.	5661	A-4-4
FLAMINCO	Huyakorn, P.S.	4630	A-3-11
FLASH	Baca, R.G.	5660	A-5-4
FLO	Vanderberg, A.	1092	A-2-6
FLOFIT	Kool, J.B.	5187	A-7-4
FLOTRA	Sagar, B.	3253	A-6-1
FLOWVEC	Li, R-M	4390	A-2-15
FLUMP	Narasimhan, T.N.	122	A-2-5
FP	Su, C.	6170	A-7-2
GLEAMS	Leonard, R.A.	3541	A-3-20

MODEL NAME	FIRST AUTHOR	IGWMC KEY	PAGE
GRWATER	Kashkuli, H.A.	3660	A-2-13
GS2	Davis, L.A.	2891	A-3-3
GS3	Davis, L.A.	2892	A-3-3
GTC	Yu, C.	5082	A-3-18
HSSWDS	Perrier, E.R.	4410	A-2-16
HYDRUS	Kool J.B.	6229	A-3-33
INFIL	Vauclin, M.	3570	A-2-12
INFGR	Craig, P.M.	4380	A-2-14
LANDFIL	Korfiatis, G.P.	4400	A-2-15
LEACHM	Wagenet, R.J.	3411	A-3-23
MATTUM	Yeh, G.T.	3375	A-5-3
MLSOIL/DFSOIL	Sjoreen, A.L.	4140	A-3-24
MMT-DPRW	Ahlstrom, S.W.	780	A-3-2
MOTIF	Guvanasen, V.	4550	A-6-3
MOUSE	Pacenka, S.	6390	A-3-22
MULTIMED	Salhotra, A.M.	5630	A-3-29
MUST	De Laat, P.J.M.	1771	A-2-6
NEWTMC	Lindstrom, F.T.	5860	A-6-6
NITRO	Kaluarachchi, J.J.	5186	A-3-26
ONESTEP	Kool, J.B.	3433	A-7-1
PESTAN	Enfield, C.G.	6130	A-4-2
PORFLOW-3D	Runchal, A.K.	3238	A-6-5
PRZM	Carsel, R.F.	4720	A-3-15
PRZMAL	Wagner, J.	5310	A-3-30
RETC	van Genuchten, M.Th.	6228	A-7-5
RITZ	Nofziger, D.L.	6620	A-3-16
RUSTIC		4721	A-3-28

MODEL NAME	FIRST AUTHOR	IGWMC KEY	PAGE
RZWQM	DeCoursey, D.G.	5850	A-3-31
SATURN	Huyakorn, P.S.	583	A-3-1
SBIR	Li, R-M	4391	A-3-9
SEEPV	Davis, L.A.	2890	A-2-9
SEEP/W (PC-SEEP)	Krahn, J.	4980	A-2-17
SESOIL	Bonazountas, M.	5039	A-3-12
SIMGRO	Querner, E.P.	5010	A-2-17
SOHYP	van Genuchten, M.Th.	6226	A-7-3
SOIL	El-Kadi, A.I.	6330	A-7-2
SOILMOP	Ross, D.L.	2062	A-2-8
SOILPROP	Mishra, S.	5183	A-7-3
SOMOF	Wesseling, J.W.	2983	A-2-10
SPLASHWATER	Milly, P.	3590	A-5-3
SUMMERS	Summers, K.	5260	A-4-3
SUTRA	Voss, C.I.	3830	A-6-1
SWACROP	Wesseling, J.G.	2550	A-2-8
SWMS-2D	Simunek, J.	6221	A-3-31
TARGET-2DU	Moreno, J.L.	4931	A-3-24
TARGET-3DU	Moreno, J.L.	4934	A-3-25
TDFD1O	Slotta, L.S.	5213	A-6-6
TOUGH	Pruess, K.	2582	A-5-1
TRACR3D	Travis, B.J.	4270	A-3-7
TRANS	Walker, W.R.	2950	A-5-2
TRIPM	Gureghian, A.B.	4081	A-3-7
TRUST	Narasimhan, T.N.	120	A-2-2
UNSAT	Khaleel, R.	6400	A-2-18
UNSAT-H	Fayer, M.J.	4340	A-2-13

MODEL NAME	FIRST AUTHOR	IGWMC KEY	PAGE
UNSAT-1	van Genuchten, M.Th.	3431	A-2-11
UNSAT1D	Gupta, S.K.	2071	A-2-7
UNSAT2	Neuman, S.P.	21	A-2-1
VADOFT	Huyakorn, P.S.	4693	A-3-26
VADOSE	Sagar, B.	3234	A-6-1
VAM2D	Huyakorn, P.S.	4690	A-3-14
VAM3D	Huyakorn, P.S.	4691	A-3-14
VIP	Stevens, D.K.	5681	A-3-30
VLEACH	Turin, J.	5690	A-4-5
VS2D/VS2DT	Lappala, E.G.	4570	A-3-10
VSAFT2	Yeh, T-C.J.	5220	A-3-27
VSAFT3	Yeh, T-C.J.	5221	A-3-27
WATERFLO	Nofziger, D.L.	6630	A-2-16

Appendix 2: Flow in the Unsaturated Zone

IGWMC Key: 21 Model Name: UNSAT2

Authors: Neuman, S.P., R. A. Feddes, and E. Bresler.
Institution of Model Development: Dept. of Hydrology and Water Resources
University of Arizona, Tucson, AZ 85721

Code Custodian: S.P. Neuman
Dept. of Hydrology and Water Resources
University of Arizona, Tucson, AZ 85721

Abstract:

UNSAT2 is a two-dimensional finite element model for horizontal, vertical, or axisymmetric simulation of transient flow in a variably saturated, nonuniform anisotropic porous medium. The governing equation is the Richard's equation expressed in terms of pressure head. Boundary conditions included are Dirichlet and Neumann, and seepage face. UNSAT2 is capable of simulating infiltration and evaporation as head-dependent conditions, determined after the fluid pressure is calculated. Evapotranspiration is simulated through user specified minimum allowed pressure head at the soil surface, maximum evaporation rate, and soil surface geometric data. User supplied input for simulation of evapotranspiration includes root zone geometric data, root effectiveness function, plant species wilting pressure, and maximum transpiration rate. The code can use both quadrilateral and triangular elements. Unsaturated hydraulic properties must be input in table form; internally, the code uses linear slopes between the data points for interpolation. UNSAT2 has a restart feature for simulating changing boundary conditions. The equation are solved with a band solver; nonlinearities are handled by a Picard iteration scheme.

Model developed for:	research (e.g. hypothesis/theory testing), general use (e.g. in field applications), demonstration/education
Documentation includes:	model theory, user's instructions, example problems, program structure and development, code listing, verification/validation
Verification/validation:	verification (analyt. solutions), laboratory data sets, field datasets (validation), synthetic datasets, code intercomparison
Peer (independent) review:	concepts, theory (math), accuracy, documentation
Availability:	public domain

Remarks:

An updated and expanded version of the documentation has been prepared by Davis and Neuman (1983, see references). The computer code of this version is available from:

Division of Waste Management
Office of Nuclear Material Safety and Safeguards
U.S. Nuclear Regulatory Commission
1717 H Street, N. W., Washington, D. C. 20555.

A debate on the representation of the seepage surface in UNSAT2 took place in Water Resources Research:

Cooley, R.L. 1983. Some New Procedures for Numerical Solution of Variably Saturated Flow Problems. Water Resourc. Res., Vol. 19(5), pp.1271-1285.

Comment by S.P. Neuman, 1985: Water Resourc. Res., Vol 21(6), p. 886. and reply by R.L. Cooley. 1985: p. 887-888.

The performance of UNSAT2 has been compared with FEMWATER, SATURN and TRUST in:

Petersen, D.M., and J.L. Wilson. 1988. Variably Saturated Flow Between Streams and Aquifers. WRRI 233, New Mexico Water Resources Res. Inst., New Mexico State Univ., Las Cruces, New Mexico.

A steady-state version of the code is available from Dr. G-T.J. Yeh, Dept. of Hydrology and Water Resources, University of Arizona, Tuscon, AZ 85721.

References:

Neuman, S. P., R. A. Feddes, and E. Bresler. 1975. Finite Element Analysis of Two-Dimensional Flow in Soils Considering Water Uptake by Roots; 1. Theory. Soil Soc. Am., Proceed. Vol. 39(2), pp. 224-230.

Feddes, R. A., S. P. Neuman, and E. Bresler. 1975. Finite Element Analysis of Two-Dimensional Flow in Soils; II. Field Applications. Soil Sci. Soc. Am., Proceed. Vol. 39(2), pp. 231-237.

Neuman, S. P., R. A. Feddes, and E. Bresler. 1974. Finite Element Simulation of Flow in Saturated-Unsaturated Soils Considering Water Uptake by Plants. 3rd Ann. Rept. Project A10-SWC-77, Hydrodynamics and Hydraulics Engineering Lab., Technion, Haifa, Israel.

Davis, L. A. and S. P. Neuman. 1983. Documentation and User's Guide: UNSAT2 - Variably Saturated Flow Model. NUREG/CR -3390, U. S. Nuclear Regulatory Commission, Washington, D.C.

IGWMC Key: 120 Model Name: TRUST

Authors: Narasimhan, T.N.

Institution of Model Development: Lawrence Berkeley Laboratory, Earth Sciences Division, University of California, Berkeley, CA 94720

Code Custodian: Narasimhan,T.N. (address see above)

Abstract:

TRUST is an integrated finite difference simulator for computation of transient pressure head distributions in multidimensional, heterogeneous, variably saturated, deformable porous media with complex geometry. Deformation of the skeleton may be nonelastic. The polygon-based model considers pressure-dependent density variations. The code calculates internally hydraulic conductivity and fluid mass capacity from intrinsic permeability, fluid viscosity, fluid density, gravitational constants, void ratio, and compressibilities. The model allows for hysteresis. The governing equations are solved by an mixed explicit-implicit scheme, using a pointwise iterative solver. Optionally, a direct solver version is available form the author. This scheme recognized that regions with small time constants might be weakly coupled, resulting in a highly effective iterative solution algorithm. All boundaries of the flow domain are handled by a general head boundary algorithm. Thus, any boundary condition is developed by manipulating a conductance term that comprises the coefficient of the head differential between interior and exterior boundary node. In addition, TRUST can handle seepage faces. The recent versions of TRUST allow both harmonic and geometric means for the conductance term and includes an algorithm for automatically generating successive time step durations.

Model developed for: research (e.g. hypothesis/theory testing), general use (e.g. in field applications), demonstration/education

Documentation includes:	model theory, user's instructions, example problems, program structure and development, verification/validation
Verification/validation:	verification (analyt.solutions), laboratory data sets, code intercomparison
Peer (independent) review:	concepts, theory (math), coding, documentation, performance
Availability:	public domain

Remarks:

The TRUST code can be coupled with the FLUX program (available from the same source) to generate a velocity field and the program MILTVL to calculate traveltimes and to generate pathlines and isochrones.

TRUST is based on the TRUMP code originally developed by A. L. Edwards at Lawrence Livermore Laboratory, Univ. of Calif, Livermore, Calif.

Modifications were made to the code to simulate flow in fractured unsaturated porous media as discussed in Wang and Narasimhan (1984; see references). These modifications include additional characteristic curves and relative permeability curves, van Genuchten formulae for matrix blocks, gamma distribution formulae for discrete fracture grid blocks, hyperbolic characteristic curves of Pickens, and a new effective area factor. The new version of TRUST uses either the existing efficient iterative solver or a new direct solution.

DYNAMIX is a code that couples a version of the program TRUMP with the geochemical code PHREEQE (Narasimhan, White and Tokunaga (1985; see user references).

TRUST-II is an updated version of the TRUST code by Narasimhan (1976) developed for the U.S. Nuclear Regulatory Commission by Battelle Pacific Northwest Laboratories (Reisenauer et Al. 1982; see references).

The TRUST code can be coupled with the FLUX program (available from the same source) to generate a velocity field and program MILTVL to calculate travel times and to generate pathlines and isochrones.

SOILGEN contains subroutines to calculate soil moisture characteristic curves based on the work of Haverkamp, van Genuchten, and Brooks and Su. The user supplies laboratory determined moisture content versus matric potential points. The code minimizes the sum squared error of the function over the experimental data. Relative hydraulic conductivity functional relationships may be determined using the Haverkamp function if experimental data is available or a method based on the Mualem theory if only moisture characteristic curve data is available.

GRIDGEN was developed to facilitate quick grid generation use with TRUST-II and supplies the data for blocks 4 and 5 of the TRUST-II code.

MLTRAN uses the method of characteristics to solve the advective transport equation with retardation. This package uses a finite element grid, therefore the original TRUST-II grid must be transformed by MLTRAN using the user supplied data. This model consists of 6 submodels that contours potential head, water content, and pressure head, generates a plot of the finite element mesh, and plots the movement of water and contaminants.

The performance of TRUST has been compared with UNSAT2, FEMWATER, and SATURN in: Petersen, D.M., and J.L. Wilson. 1988. Variably Saturated Flow Between Streams and Aquifers. WRRI 233, New Mexico Water Resources Res. Inst., New Mexico State Univ., Las Cruces, New Mexico.

References:

Narasimhan, T.N. and P.A. Witherspoon. 1976. An Integrated Finite Difference Method for Fluid Flow in Porous Media. Water Resources Research, Vol. 12(1), pp. 57- 64.

Narasimhan, T.N. 1975. A Unified Numerical Model for Saturated-Unsaturated Ground-Water Flow. Ph. D. Dissertation, University of California, Berkeley, Calif.

Narasimhan, T.N. and P.A. Witherspoon. 1977. Numerical Model for Saturated-Unsaturated Flow in Deformable Porous Media; I. Theory. Water Resources Research, Vol. 13(3); pp. 657-664.

Narasimhan, T.N., P.A. Witherspoon, and A.L. Edwards. 1978. Numerical Model for Saturated-Unsaturated Flow in Deformable Porous Media; II. The Algorithm. Water Resources Research, Vol. 14(2), pp. 255-261.

Narasimhan, T.N., and P.A. Witherspoon. 1978. Numerical Model for Saturated-Unsaturated Flow in Deformable Porous Media; III. Applications. Water Resources Research, Vol. 14(6), pp. 1017-1034.

Narasimhan, T.N., and W.A. Palen. 1981. Interpretation of a Hydraulic Fracturing Experiment, Monticello, South Carolina. AGU Geophysical Research Letters, Vol. 8(5), pp. 481-484.

Narasimhan, T.N. 1979. The Significance of the Storage Parameter in Saturated-Unsaturated Groundwater Flow. Water Resources Research, Vol. 15(3), pp. 569-576.

Reisenauer, A.E., K.T. Key, T.N. Narasimhan, and R.W. Nelson. 1982. TRUST: A Computer Program for Variably Saturated Flow in Multidimensional, Deformable Media. NUREG/CR-2360, U.S. Nuclear Regulatory Commission, Washington, D.C.

Wang, J.S.Y., and T.N. Narasimhan. 1984. Hydrologic Mechanisms Governing Fluid Flow in Partially Saturated Fractured, Porous Tuff at Yucca Mountain. Lawrence Berkeley Laboratory, University of Calif., Berkeley, Calif.

Narasimhan, T.N., and S.J. Dreiss. 1986. A Numerical Technique for Modeling Transient Flow of Water to a Soil Water Sampler. Soil Science, Vol. 14(3), pp. 230-236.

McKeon, T.J., S.W. Tyler, D.W. Mayer, and A.E. Reisenauer. 1983. TRUST-II Utility Package: Partially Saturated Soil Characterization, Grid Generation, and Advective Transport Analysis. NUREG/CR-3443, U.S. Nuclear Regulatory Commission, Washington, D.C.

IGWMC Key: 122 Model Name: FLUMP

Authors: Narasimhan, T.N. (1), and S.P. Neuman (2)
Institution of Model Development: (1) See code custodian; (2) University of Arizona, Tucson, Arizona

Code Custodian: T.N. Narasimhan
Lawrence Berkeley Laboratory, Earth Sciences Div.
University of Calif., Berkeley, CA 94720

Abstract:

FLUMP is a finite element program for the computation of steady and nonsteady, two-dimensional areal or cross-sectional pressure-head distribution in heterogeneous, anisotropic, variably saturated porous media with complex geometry.

Model developed for:	research (e.g. hypothesis/theory testing), general use (e.g. in field applications), demonstration/education
Documentation includes:	model theory, user's instructions, example problems, verification/validation
Verification/validation:	verification (analyt.solutions)
Peer (independent) review:	concepts, theory (math)
Availability:	public domain

Remarks:

FLUMP is especially suited for problems with moderate or high saturation. Some stability problems may be encountered while applying code to desiccated soils.

A version of FLUMP allowing for subsidence due to pumping in a multi-layered aquifer system has been developed by S.P. Neuman, C. Preller, and T.N. Narasimhan. This code is called FLUMPS and is annotated under IGWMC-key # 00025.

FLUMP is based on a computer program for temperature distributions in multi-dimensional systems, originally developed by A.L. Edwards, Lawrence Livermore Laboratory, University of California, Livermore, in 1969. The original code, TRUMP, has been annotated as IGWMC-key # 04030.

References:

Neuman, S.P. and T.N. Narasimhan. 1975. Mixed Explicit-Implicit Iterative Finite Element Scheme for Diffusion Type Problems; I. Theory. Rept. 4405, Lawrence Berkeley Laboratory (also published in Internat. J. for Numerical Methods in Engineering).

Narasimhan, T.N., S.P. Neuman, and A.L. Edwards. 1975. Mixed Explicit-Implicit Iterative Finite Element Scheme for Diffusion-Type Problems; II. Solution Strategy and Examples. Rept. 4406, Lawrence Berkeley Laboratory, Berkeley, Calif. (also published in Internat. J. for Numerical Methods in Engineering).

Narasimhan, T.N., S.P. Neuman, and P.A. Witherspoon. 1978. Finite Element Method for Subsurface Hydrology Using a Mixed Explicit-Implicit Iterative Scheme. Water Resources Research, Vol. 14(5), pp. 863-877.

Neuman, S.P., T.N. Narasimhan, and P.A. Witherspoon. 1976. Application of Mixed Explicit-Implicit Finite Element Method to Nonlinear Diffusion-Type Problems. In: Proceed. Internat. Conf. on Finite Elements in Water Resources, Princeton University, Princeton, New Jersey, July 12-16, 1976.

IGWMC Key: 1092 Model Name: FLO
Authors: Vandenberg, A.
Institution of Model Development: National Hydrology Research Institute
Inland Waters Directorate, Ottawa, Ontario, Canada
Code Custodian: Vandenberg, A.
National Hydrology Research Institute, Inland Waters Directorate
Ottawa, K1A OE7 Ontario, Canada
Abstract:

FLO simulates the elements of the hydrological cycle directly influenced by soil and surface drainage improvements. Total discharge from a drained plot includes surface runoff, and drain discharge is estimated. Detailed accounts of unsaturated flow is considered, including capillary forces and evapotranspiration.

Model developed for: research (e.g. hypothesis/theory testing), general use (e.g. in field applications)
Documentation includes: model theory, user's instructions, example problems
Availability: public domain

References:

Vandenberg, A. 1985. A Physical Model of Vertical Infiltration, Drain Discharge and Surface Runoff. National Hydrology Research Institute, Inland Water Directorate, Ottawa, Canada.

IGWMC Key: 1771 Model Name: MUST (Model for Unsaturated flow above a Shallow water Table)
Authors: De Laat, P.J.M.
Institution of Model Development: International Institute for Hydraulic & Environm. Eng.
Delft, The Netherlands
Code Custodian: De Laat, P.J.M.
International Inst. for Hydraulic & Env. Eng.
Oude Delft 95, Delft, The Netherlands
Abstract:

MUST is a finite difference model which simulates one-dimensional vertical, unsaturated groundwater flow, evapotranspiration, plant uptake, and interception of precipitation by plants.

Model developed for: research (e.g. hypothesis/theory testing), general use (e.g. in field applications)
Documentation includes: model theory, user's instructions, example problems, program structure and development, code listing, verification/validation
Verification/validation: verification (analyt.solutions), laboratory data sets, field datasets (validation)
Peer (independent) review: concepts, theory (math)
Availability: restricted public domain

Remarks:

MUST is an extensively modified version of the code UNSAT by P.J.M. De Laat. These modifications especially concern the way evapotranspiration is treated and include interception of precipitation.

References:

De Laat, P.J.M. 1985. Must, A Simulation Model for Unsaturated Flow. Report Series No. 16, Internat. Inst. for Hydraulic and Environm. Eng., Delft, The Netherlands.

De Laat, P.J.M. 1985. *Simulation of Evapotranspiration and Sprinkling with MUST.* H20, Vol. 18, pp. 363-367. (in Dutch).

IGWMC Key: 2071 Model Name: UNSAT1D

Authors: Gupta, S.K., C.S. Simmons, F.W. Bond, and C.R. Cole

Institution of Model Development: Battelle Pacific NW Laboratories, Richland, Washington

Code Custodian: Simmons, C.S.
Battelle Pacific NW Laboratories, P.O. Box 999, Richland, WA 99352

Abstract:

UNSAT1D is a fully implicit one-dimensional finite difference model for simulation of transient vertical unsaturated flow in homogeneous, heterogeneous or layered soil profile. The program simulates infiltration, vertical seepage, and plant uptake by roots as function of the hydraulic properties of soil, soil layering, root growth characteristics, evapotranspiration rates, and frequency, rate, and amount of precipitation and/or irrigation. It can handle boundary conditions related to rain, sprinkler or flood irrigation, or constant head conditions in the upper boundary. The lower boundary can be the water table, dynamic or quasi-dynamic, or unit gradient. The model estimates groundwater recharge, irrigation and consumptive use of water, return flows, etc.

Model developed for:	research (e.g. hypothesis/theory testing), general use (e.g. in field applications)
Documentation includes:	model theory, user's instructions, example problems, code listing, verification/validation
Verification/validation:	verification (analyt.solutions), code intercomparison
Peer (independent) review:	concepts, theory (math), documentation
Availability:	early version is public domain; EPRI version is proprietary and available with license

Remarks:

A version with updated documentation is available from EPRI (Electric Power Research Institute, P.O. Box 50490, Palo Alto, CA 94303.

References:

Gupta, S.K., K.K. Tanji, D.R. Nielsen, J.W. Biggar, C.S. Simmons, and J.L. MacIntyre. 1978. Field Simulation of Soil-Water Movement with Crop Water Extraction. Water Science and Engineering Paper No. 4013, Univ. of Calif. Dept. of Land, Air and Water Resources, Davis, Calif.

Bond, F.W., C.R. Cole and P.J. Gutknecht. 1984. Unsaturated Groundwater Flow Model (UNSAT1D) Computer Code Manual. CS-2434-CCM, Electric Power Research Inst., Palo Alto, Calif.

Battelle Pacific Northwest Lab. 1984. Comparison of Two Groundwater Flow Models - UNSAT1D and HELP. EPRI CS-3695, Electric Power Research Inst., Palo Alto, Calif.

IGWMC Key: 2062 Model Name: SOILMOP

Authors: Ross, D.L., and H.J. Morel-Seytoux

Institution of Model Development: Colorado State University
Dept. of Civil Eng., Fort Collins, Colorado

Code Custodian: Morel-Seytoux, H.J.
Colorado State University, Dept. of Civil Eng.
Fort Collins, CO 80523

Abstract:

SOILMOP is an analytical model to predict ponding time, infiltration rate and amount, and water content profiles under variable rainfall conditions. The model solves a one-dimensional flow equation in a homogeneous soil. Air phase is also included.

Model developed for: research (e.g. hypothesis/theory testing), general use (e.g. in field applications)

Documentation includes: model theory, user's instructions, example problems, program structure and development, code listing

Availability: public domain

References:

Ross, D.L. and H.J. Morel-Seytoux. 1982. User's Manual for SOILMOP: A Fortran IV Program for Prediction of Infiltration and Water Content Profiles Under Variable Rainfall Conditions. Interim Report for FY 1981-1982, DER-82-DLR-HJM45, Dept. of Civil Eng., Colorado State Univ., Fort Collins, Colorado.

Morel-Seytoux, H.J. 1979. Analytical Results for Predictions of Variable Rainfall Infiltration, Hydrowar Program, CEP 79-80HJM37, Dept. of Civil Eng., Colorado State Univ., Fort Collins, Colorado.

IGWMC Key: 2550 Model Name: SWACROP

Author: Wesseling, J.G., P. Kabat, B.J. van den Broek, and R.A. Feddes

Institution of Model Development: Winand Staring Centre
Wageningen, The Netherlands

Code Custodian: Winand Staring Centre, Dept. of Agrohydrology
Wageningen, The Netherlands

Abstract:

SWACROP (Soil WAter and CROP production model) is a transient one-dimensional finite difference model for simulation of the unsaturated zone, which incorporates water uptake by roots. The soil profile is divided into several layers (containing one or more compartments of variable thickness) having different physical properties. The partial differential equation for flow in the unsaturated system is solved using a implicit finite difference scheme. An explicit linearization of the hydraulic conductivity and soil water capacity is used. Knowing the initial conditions (i.e. water content or pressure head distribution profile) and top and bottom boundary conditions, the system of equations for all the compartments is solved for each (variable) timestep by applying the so-called Thomas tri-diagonal algorithm. The iteration procedure within each timestep allows calculation of all water balance terms for each time period selected.

For the top boundary condition data on rainfall, potential soil evaporation and potential transpiration are required. When the soil system remains unsaturated, one of three bottom boundary conditions can be used:

pressure head, zero flux, or free drainage. When the lower part of the system remains saturated, one can either give the ground-water level or the flux through the bottom of the system as input. In the latter case the ground-water level is computed. The rate of vegetation growth, both potential and actual can be simulated in the crop growth submodel linked to the main water model in a complex dynamic way. However, both models can easily be run separately.

Model developed for:	research (e.g. hypothesis/theory testing), general use (e.g. in field applications)
Documentation includes:	model theory, user's instructions, example problems, code listing
Peer (independent) review:	concepts, theory (math)
Availability:	restricted public domain; purchase

References:

Feddes, R.A., P.J. Kowalik and H. Zaradny. 1978. Simulation of Field Water Use and Crop Yield. Centre for Agriculture. Publ. and Doc. (PUDOC), Wageningen, The Netherlands.

Belmans, C., J.G. Wesseling and R.A. Feddes. 1981. Simulation Model of the Water Balance of a Cropped Soil Providing Different Types of Boundary Conditions (SWATRE). Nota 1257, Inst. of Land and Water Management Research (ICW), Wageningen, The Netherlands.

Belmans, C., J.G. Wesseling and R.A. Feddes. 1983. Simulation Model of the Water Balance of a Cropped Soil, SWATRE. J. of Hydrology, Vol. 63(3/4), pp. 271-286.

Wesseling, J.G., P. Kabat, B.J. van den Broek and R.A. Feddes. 1989. SWACROP: Simulating the dynamics of the unsaturated zone and water limited crop production. Winand Staring Centre, Department of Agrohydrology, Wageningen, The Netherlands.

IGWMC Key: 2890 Model Name: SEEPV

Authors: Davis, L.A.

Institution of Model Development: Water, Waste and Land, Inc.
Fort Collins, Colorado

Code Custodian: Davis, Lyle A.
Water, Waste and Land, Inc.
1311 S. College Avenue, Fort Collins, CO 80524

Abstract:

SEEPV is a transient finite difference model to simulate vertical seepage from a tailings impoundment in variably saturated flow system; the program takes into consideration the interaction between an impoundment liner and the underlying aquifer.

Model developed for:	general use (e.g. in field applications)
Documentation includes:	model theory, user's instructions, code listing,
Verification/validation:	verification (analyt.solutions)
Peer (independent) review:	concepts, theory (math)
Availability:	public domain

References:

Davis, L.A. 1980. Computer Analysis of Seepage and Groundwater Response Beneath Tailing Impoundments. Report Grant NSF/RA-800054, Nat. Science Foundation, Washington, D.C.

IGWMC Key: 2983 Model Name: SOMOF
Authors: Wesseling, J.W.
Institution of Model Development: Delft Hydraulics Laboratory
Emmeloord, The Netherlands
Code Custodian: Wesseling, J.W.
Delft Hydraulics Laboratory
P.O. Box 152, 8300 AD Emmeloord, The Netherlands

Abstract:

SOMOF is s finite difference model for the simulation of transient unsaturated soil moisture flow in a vertical profile. The model handles various processes, including infiltration from precipitation, capillary forces, evapotranspiration, gravity drainage, ponding, and plant uptake.

Model developed for: research (e.g. hypothesis/theory testing), general use (e.g. in field applications)
Documentation includes: model theory, user's instructions, example problems
Availability: proprietary, license

Remarks:
SOMOF has been applied for a verification study of the "Black-Box" model, initially used in the PAWN (Policy Analysis of the Water Management in The Netherlands) study.

References:
The Soil Moisture Zone in a Physically Based Hydrologic Model (PREDIS). Adv. Water Resources.

IGWMC Key: 3370 Model Name: FEMWATER/FECWATER
Authors: Yeh, G.T., and D.S. Ward
Institution of Model Development: Oak Ridge National Laboratory
Oak Ridge, Tennessee
Code Custodian: G.T. Yeh
Penn State University, Dept. of Civil Eng.
225 Sackett Bldg, University Park, PA 16802

Abstract:

FEMWATER is a two-dimensional finite element model to simulate transient, cross-sectional flow in saturated-unsaturated anisotropic, heterogeneous porous media. The model is designed to treat both point sources/sinks and non-point sources/sinks, and to handle a wide variety of non-steady state boundary conditions, including a moving water-table and seepage faces. It allows three alternative approximations for the time derivative, has three options for estimating the non-linear matrix, and a direct and an iterative matrix solution option. Furthermore, the program includes automatic time-step adjustment and has an option to consider axisymmetric problems.

Model developed for: research (e.g. hypothesis/theory testing), general use (e.g. in field applications)
Documentation includes: model theory, user's instructions, example problems, program structure and development, code listing, verification/validation
Verification/validation: verification (analyt.solutions), laboratory data sets
Peer (independent) review: concepts, theory (math), documentation
Availability: public domain

Remarks:

FEMWATER is an extensively modified and expanded version of a finite-element Galerkin model developed by Reeves and Duguid (1975; see references).

FECWATER is a slightly updated version of the FEMWATER version of 1980. A revised version of FEMWATER was written by G.T. Yeh (1987; see references)

References:

Yeh, G.T. and D.S. Ward. 1980. FEMWATER: A Finite-Element Model of Water Flow Through Saturated-Unsaturated Porous Media. ORNL-5567. Oak Ridge National Laboratory, Oak Ridge, Tennessee.

Yeh, G.T. 1987. FEMWATER: A Finite Element Model of Water Flow through Saturated-Unsaturated Porous Media First Revision. ORNL 5567/R1, Oak Ridge Nat. Lab., Oak Ridge, Tennessee.

Reeves, M., and J.O. Duguid. 1975. Water Movement through Saturated-Unsaturated Porous Media: A Finite Element Galerkin Model. ORNL-4927, Oak Ridge National Lab., Oak Ridge, Tennessee.

Yeh, G.T. and R.H. Strand. 1982. FECWATER: User's Manual of a Finite-Element Code for Simulating Water Flow Through Saturated-Unsaturated Porous Media. ORNL/TM 7316, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

Yeh, G.T., 1982. Training Course No. 1: The Implementation of FEMWATER (ORNL-5567) Computer Program. NUREG/CR-2705, U.S. Nuclear Regulatory Commission, Washington, D.C.

IGWMC Key: 3431 Model Name: UNSAT-1

Author: Van Genuchten, M.Th.

Institution of Model Development: Water Resources Program, Dept. of Civil Eng.
Princeton University, Princeton, New Jersey

Code Custodian: Van Genuchten, M.
USDA Salinity Laboratory
4500 Glenwood Drive, Riverside, CA 92501

Abstract:

UNSAT-1 is a Hermetian finite element solution to the Richards' equation for transient one-dimensional, variably saturated flow in layered soils. The model can handle both abrupt layering and smoothly changing profile properties.

Model developed for:	research (e.g. hypothesis/theory testing)
Documentation includes:	model theory, user's instructions, example problems, code listing, verification/validation
Verification/validation:	verification (analyt.solutions)
Availability:	public domain

Remarks:

This model is available from the International Ground Water Modeling Center, Colorado School of Mines, Golden, CO 80401.

References:

Van Genuchten, M.Th. 1978. Numerical Solutions of the One-Dimensional Saturated/Unsaturated Flow Equation. Rept. 78-WR-9, Water Resources Progr., Dept. of Civil Engineering, Princeton University, Princeton, New Jersey.

IGWMC Key: 3570 Model Name: INFIL

Author: Vauclin, M.

Institution of Model Development: Institute de Mecanique de Grenoble
St. Martin D'Heres, France

Code Custodian: M. Vauclin
Institute de Mecanique de Grenoble
BP 68, 38402 St. Martin D'Heres - Cedex France

Abstract:

INFIL is a finite difference model which solves for ponded infiltration into a deep homogeneous soil. The model is based on the Philip series solution (1957) of a one-dimensional form of the Richards equation. Output includes water content profile and amount and rate of infiltration at different simulation times. The program, which requires the soil properties to be expressed in mathematical form, is designed to accommodate three different sets of these functions. They include the four parameter function of Vauclin (1979), the three parameter functions of Brutseart (1966 and 1967), and the two parameter function of Brooks and Corey (1964). A modified version by A.I. El-Kadi also includes a van Genuchten function (1978).

Model developed for:	research (e.g. hypothesis/theory testing), general use (e.g. in field applications), demonstration/education
Documentation includes:	model theory, user's instructions, example problems, code listing, verification/validation
Verification/validation:	verification (analyt.solutions), laboratory data sets
Peer (independent) review:	concepts, theory (math)
Availability:	proprietary, purchase

Remarks:

Both the original FORTRAN and modified BASIC versions are available from the International Ground Water Modeling Center (IGWMC), Colorado School of Mines, Golden, CO 80401.

References:

El-Kadi, A.I. 1983. INFIL: A Fortran IV Program to Calculate Infiltration Rate and Amount and Water Content Profile at Different Times. FOS-20, International Ground Water Modeling Center, Holcomb Research Institute, Indianapolis, Indiana.

Vauclin, M., R. Haverkamp and G. Vachaud. 1979. Resolution Numerique D'une Equation De Diffusion Non Linearie. Presses Universitaires De Grenoble, Grenoble, France.

IGWMC Key: 3660 Model Name: GRWATER
Authors: Kashkuli, H.A.
Institution of Model Development: Colorado State University
Dept. of Civil Eng., Fort Collins, Colorado
Code Custodian: Daniel K. Sunada
Dept. of Civil Eng., Colorado State University
Fort Collins, CO 80523

Abstract:

GRWATER is a finite difference model to predict the decline of ground water mounds developed under recharge in an isotropic, heterogeneous water table aquifer. The model has two modules, one for transient one-dimensional unsaturated flow above the water table which handles infiltration and evapotranspiration, and one for transient two-dimensional horizontal saturated flow in the aquifer.

Model developed for: research (e.g. hypothesis/theory testing)
Documentation includes: model theory, user's instructions, example problems, code listing, verification/validation
Verification/validation: verification (analyt.solutions)
Peer (independent) review: concepts, theory (math)
Availability: public domain

Remarks:
The program GRWATER consists of two subprograms, UNSATF for the unsaturated zone and LINKFLO for the water table aquifer. LINKFLO is described under IGWMC-Key 2670

References:
Kashkuli, H.A. 1981. A Numerical Linked Model for the Prediction of the Decline of Groundwater Mounds Developed under Recharge. Ph.D. Thesis, Colorado State Univ., Fort Collins, Colorado.

IGWMC Key: 4340 Model Name: UNSAT-H
Authors: Fayer, M.J., and G.W. Gee
Institution of Model Development: Battelle Pacific Northwest Laboratory
Richland, Washington
Code Custodian: Fayer, M.J.
Battelle Pacific Northwest Laboratory
P.O. Box 999, Richland, WA 99352

Abstract:

UNSAT-H is a one-dimensional finite difference model for simulation of vertical unsaturated soil moisture flow. It simulates infiltration, drainage, redistribution, surface evaporation and plant water uptake from soil. The model's numerical technique is specially designed for arid zones characterized by very dry soils similar to the Hanford site (Washington).

Model developed for: general use (e.g. in field applications)
Documentation includes: model theory, user's instructions, example problems, program structure and development, code listing, verification/validation
Verification/validation: verification (analyt.solutions)
Peer (independent) review: concepts, theory (math), documentation
Availability: public domain

Remarks:

UNSAT-H is based on a computer code that was developed by Gupta et al (1978; see references) to model soil water movement with concurrent crop water extraction. A version of the Gupta et al. (1978) code, UNSAT1D (IGWMC key # 2071), was documented by Bond et al. (1984; see references).

References:

Fayer, M.J. and G.W. Gee. 1985. UNSAT-H: An Unsaturated Soil Water Flow Code for Use at the Hanford Site: Code Documentation. PNL-5585, Battelle Pacific Northwest Lab., Richland, Wash.

Gupta, S.K., K.K. Tanji, D.R. Nielsen, J.W. Biggar, C.S. Simmons, and J.L. MacIntyre. 1978. Field Simulation of Soil-Water Movement with Crop Water Extraction. Water Science and Engineering Paper No. 4013, Univ. of Calif. Dept. of Land, Air and Water Resources, Davis, Calif.

Bond, F.W., C.R. Cole and P.J. Gutknecht. 1984. Unsaturated Groundwater Flow Model (UNSAT1D) Computer Code Manual. CS-2434-CCM, Electric Power Research Inst., Palo Alto, Calif.

IGWMC Key: 4380 Model Name: INFGR

Authors: Craig, P.M., and E.C. Davis

Institution of Model Development: University of Tennessee
Knoxville, Tennessee

Code Custodian: Davis, E.C.
Oak Ridge National Lab., Environm. Sciences Div.
Oak Ridge, Tennessee 37830

Abstract:

INFGR is one-dimensional model to estimate the infiltration rate using the Green and Ampt equation. The compression method is used to estimate infiltration during low rainfall periods. The model works well for determining infiltration but performs poorly in determining soil moisture content.

Model developed for: research (e.g. hypothesis/theory testing), general use (e.g. in field applications)

Documentation includes: user's instructions, code listing

Availability: public domain

Remarks:

The INFGR has been used in conjunction with FEWA (Oak Ridge National Lab.; see IGWMC Key # 3373) to estimate groundwater recharge in a pollution problem (Graig and Davis, 1985; see references).

References:

Craig, P.M. and E.C. Davis. 1985. Application of the Finite Element Groundwater Model FEWA to the Engineered Test Facilities. Oak Ridge National Lab., Publ. No. 2581, Environmental Sciences Division, Oak Ridge, Tenn.

IGWMC Key: 4390 Model Name: FLOWVEC
Authors: Li, R-M., K.G. Eggert, and K.Zachmann
Institution of Model Development: Simons, Li and Associates, Inc.
Fort Collins, Colorado

Code Custodian: Ruh-Ming Li
Simons, Li and Associates, Inc.
P.O. Box 1816, Fort Collins, CO 80522

Abstract:

FLOWVEC utilizes a vector processor for solving three-dimensional, variably saturated flow problems. The model employs a finite difference technique in the formulation of the governing equations and a block implicit scheme in the solution.

Model developed for: research (e.g. hypothesis/theory testing)
Documentation includes: model theory, user's instructions, example problems, program structure and development, code listing, verification/validation
Verification/validation: verification (analyt.solutions)
Peer (independent) review: concepts, theory (math)
Availability: public domain

References:

Li, R-M, K.G. Eggert and K. Zachmann. 1983. Parallel Processor Algorithm for Solving Three-Dimensional Ground Water Flow Equations. National Science Foundation, Washington, D.C.

IGWMC Key: 4400 Model Name: LANDFIL
Authors: Korfiatis, G.P.
Institution of Model Development: Rutgers University
Civil and Environmental Eng., New Brunswick, New Jersey

Code Custodian: George P. Korfiatis
Stevens Institute of Technology, Department of Civil Engineering
Hoboken, NJ 07030

Abstract:

LANDFIL simulates the movement of moisture through the unsaturated zone using a finite difference solution for the one-dimensional flow equation. Conditions simulated are pertinent to landfills. Precipitation, evapotranspiration and redistribution are considered. Both lined and unlined landfills may be simulated.

Model developed for: research (e.g. hypothesis/theory testing)
Documentation includes: model theory, user's instructions, example problems, code listing
Peer (independent) review: concepts, theory (math)
Availability: public domain

References:

Korfiatis, G.P. 1984. Modeling the Moisture Transport through Solid Waste Landfills. PhD Thesis, Rutgers University, The State University of New Jersey, New Brunswick, New Jersey.

IGWMC Key: 4410 Model Name: HSSWDS
Authors: Perrier, E.R., and A.C. Gibson
Institution of Model Development: Water Resources Engineering Group Environmental Lab.
U.S. Army Engineer Waterways Experiment Station
Vicksburg, Mississippi 39185
Code Custodian: Landreth, R.E.
Municipal Environmental Research Laboratory
Solid and Hazardous Waste Research Div.
U.S. Environmental Protection Agency
Cincinnati, OH 45268

Abstract:

HSSWDS is a one-dimensional, deterministic, water budget model to estimate the amount of moisture percolation through different types of landfill. The model was adapted from the CREAMS model (IGWMC key # 3540) and includes recharge from precipitation, surface runoff and evapotranspiration.

Model developed for: general use (e.g. in field applications)
Documentation includes: model theory, user's instructions, example problems, code listing
Availability: public domain

References:

Perrier, E.R. and A.C. Gibson. 1982. Hydraulic Simulation of Solid Waste Disposal Sites. Office of Solid Waste and Emergency Response, U.S. Environmental Protection Agency, Washington, D.C.

IGWMC Key: 6630 Model Name: WATERFLO
Authors: Nofziger, D.L.
Institution of Model Development: Univ. of Florida, Soil Science Dept.
Gainesville, Florida
Code Custodian: Dennis Watson, IFAS - Software Support, University of Florida
Building 664, Room 203, Gainesville, FL 32611

Abstract:

The WATERFLO model is based on a finite difference solution of the one-dimensional nonlinear Richards equation for simulation of water movement through homogeneous soils. The interactive microcomputer program can accommodate finite and semi-finite soil systems. It provides for the following boundary conditions at the soil surface: constant potential, constant flux density, rainfall or sprinkler infiltration rate, and mixed type (flux and potential boundary condition).

Model developed for: research (e.g. hypothesis/theory testing), general use (e.g. in field applications), demonstration/education
Documentation includes: model theory, user's instructions, example problems, verification/validation
Verification/validation: verification (analyt.solutions), laboratory data sets, field datasets (validation)
Peer (independent) review: concepts, theory (math)
Availability: public domain

References:

Nofziger, D.L. 1985. Interactive Simulation of One-Dimensional Water Movement in Soils: User's Guide. Circular 675, Software in Soils Science, Florida Coop. Extension Service, Univ. of Florida, Gainesville, Florida.

IGWMC Key: 4980 Model Name: SEEP/W (PC-SEEP)
Authors: Krahn, J., D.G. Fredlund, L. Lam, and S.L. Barbour
Institution of Model Development: Geo-Slope Programming Ltd.
Calgary, Alberta, Canada
Code Custodian: J. Krahn
Geo-Slope Programming Ltd.
7927 Silver Springs Road NW, Calgary, Alberta, Canada T3B 4K4

Abstract:

SEEP/W is an interactive finite element program for simulating steady-state and transient 2D cross-sectional flow in both the saturated and unsaturated zones. It can simulate surface infiltration and evapotranspiration and handle internal drains. SEEP/W is designed to analyze seepage through earth dams, watertable location and fluctuations, and mounding of the watertable underneath a leaking waste pond. The model computes nodal pore-water pressures, hydraulic heads, velocities, flow directions and flow gradients. It includes postprocessors for finite element mesh plots, head contours and velocity vector plots. SEEP/W provides options to use either an in-core or an out-of-core iterative solver for the nonlinear flow equations.

Model developed for: general use (e.g. in field applications)
Documentation includes: model theory, user's instructions, example problems
Availability: proprietary, purchase

Remarks:

SEEP/W consists of three group of programs: 1) data input simulation preprocessor PROMSEEP; 2) main processors SEEPSS (steady-state, in-core solver), SEEPTR (transient and steady-state, in core solver), and SEEPOC (steady-state, out-of-core solver), and 3) post-processors DOT20 (mesh plots), DOT21 (contour plots), and DOT22 velocity vector plots).

References:

Krahn, J., D.G. Fredlund, L. Lam, and S.L Barbour. 1989. PC-SEEP: A Finite Element Program for Modelling Seepage. Geo-Slope Programming, Ltd., Calgary, Alberta, Canada.

IGWMC Key: 5010 Model Name: SIMGRO
Authors: Querner, E.P.
Institution of Model Development: Inst. for Land and Water Management Research (ICW)
Wageningen, The Netherlands
Code Custodian: E.P. Querner
Inst. for Land and Water Management Research (ICW)
P.O. Box 35, 6700 AA Wageningen, The Netherlands

Abstract:

SIMGRO (SIMulation of GROundwater flow and surface water levels) simulates flow in the saturated zone, the unsaturated zone, and a surface water system. The saturated zone model consists of a quasi-threedimensional finite element model with an implicit calculation scheme. The unsaturated zone is modeled by means of two reservoirs, one for the root zone and one for the subsoil. The root zone is treated using a water balance model and includes storage and resulting change in phreatic level, capillary rise, percolation and evapotranspiration. The surface water system, representing a network of small channels, is considered as a single reservoir with criteria for water supply, discharge, water level control, and extraction for sprinkling.

Model developed for: general use (e.g. in field applications)
Documentation includes: model theory, user's instructions, example problems
Availability: proprietary, purchase

References:

Querner, E.P. 1986. An Integrated Surface and Ground-water Flow Model for the Design and Operation of Drainage Systems. In: Proceed. Internat. Conf. on Hydraulic Design in Water Resources Engineering: Land Drainage, Southampton, UK, April 16-18, 1986, pp. 101-108. Report 15, Inst. for Land and Water Management Research (ICW), Wageningen, The Netherlands.

IGWMC Key: 6400 Model Name: UNSAT

Authors: Khaleel, R., and T-C.J. Yeh
Institution of Model Development: New Mexico Inst. of Mining and Technology
Dept. of Geoscience, Socorro, New Mexico
Code Custodian: Khaleel, R.
New Mexico Inst. of Mining and Technology
Dept. of Geoscience, Socorro, NM 87901

Abstract:

UNSAT is a Galerkin finite element model for solving the one-dimensional, transient flow equation in unsaturated porous media. It estimates the rate of infiltration into soil as well as the moisture distribution following infiltration. Both differential and cumulative mass balance errors are given to illustrate accuracy of the numerical scheme.

Model developed for: general use (e.g. in field applications), demonstration/education
Documentation includes: model theory, user's instructions, example problems, program structure and development, code listing, verification/validation
Verification/validation: verification (analyt.solutions), laboratory data sets
Peer (independent) review: concepts, theory (math)
Availability: public domain

References:

Khaleel, R., and T.-C. Yeh. 1985. A Galerkin Finite Element Program for Simulating Unsaturated Flow in Porous Media. Ground Water, Vol. 23(1), pp. 90-96.

Appendix 3: Flow and Solute Transport in the Unsaturated Zone

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IGWMC Key: 583 Model Name: SATURN
Authors: Huyakorn, P.S., S.D. Thomas, J.W. Mercer, and B.H. Lester
Institution of Model Development: GeoTrans, Inc., Sterling, Virginia

Code Custodian: David Ward, GeoTrans, Inc.
46050 Manekin Plaza, Suite 100, Sterling, VA 22170

Abstract:

SATURN (SATurated-Unsaturated flow and RadioNuclide transport) is a two-dimensional finite element model to simulate transient, single phase fluid flow and advective-dispersive transport of radionuclides and other contaminants in fully or partially saturated, anisotropic, heterogeneous porous media. The flow problem is solved using the Galerkin method to approximate the governing equation, and either the Picard or Newton-Raphson iterative techniques to treat material nonlinearities. It uses the upstream-weighted residual method to treat the transport equation.

Model developed for:	general use (e.g. in field applications), demonstration/education
Documentation includes:	model theory, user's instructions, example problems, code listing verification/validation
Verification/validation:	verification (analyt.solutions), laboratory data sets, code intercomparison
Peer (independent) review:	concepts, theory (math)
Availability:	proprietary, license

Remarks:

Nodal coordinates for SATURN may be generated by SATURN itself (for simple rectangular geometry) or by STRPGN, a separate mesh generator.

References:

Huyakorn, P.S. and S.D. Thomas. 1984. Techniques for Making Finite Elements Competitive in Modeling Flow in Variably Saturated Porous Media. Water Resources Research, Vol. 20(8), pp. 1099-1115.

Huyakorn, P.S., J.W. Mercer and D.S. Ward. 1985. Finite Element Matrix and Mass Balance Computational Schemes for Transport in Variably Saturated Porous Media. Water Resources Research, Vol. 21(3), pp. 346-358.

Huyakorn, P.S., S.D. Thomas, J.W. Mercer, and B.H. Lester. 1983. SATURN: A Finite-Element Model for Simulating Saturated-Unsaturated Flow and Radioactive Nuclide Transport. Techn. Rept. Submitted By GeoTrans, Inc. to Electric Power Research Inst., Palo Alto, Calif.

Huyakorn, P.S., V.M. Guvanasen, and T.D. Wadsworth. 1985. MGC-SATURN: Moisture Movement and Groundwater Components of the SATURN Code. Techn. Report by GeoTrans, Inc. for Electric Power Research Inst., Palo Alto, Calif.

IGWMC Key: 780 Model Name: MMT-DPRW
Authors: Ahlstrom, S.W., H.D. Foote, and R.J. Serne
Institution of Model Development: Battelle Pacific NW Laboratories
Richland, Washington
Code Custodian: J.F. Washburn
Battelle Pacific NW Laboratories
P.O. Box 999, Richland, WA 99352

Abstract:

MMT-DPRW is a three-dimensional model for simulation of transient saturated and unsaturated flow and multi-component mass transport in heterogeneous, anisotropic porous media. The model is based on a finite difference approximation of flow and advective transport of non-conservative species, and a discrete particle random walk technique for the simulation of hydrodynamic dispersion.

Model developed for: research (e.g. hypothesis/theory testing), general use (e.g. in field applications)
Documentation includes: model theory, user's instructions, example problems, verification/validation
Verification/validation: verification (analyt.solutions)
Peer (independent) review: concepts, theory (math)
Availability: public domain

Remarks:
Updated one-dimensional version is available as MMT-1D. (see IGWMC Key # 0781).

References:
Ahlstrom, S.W. and H.P. Foote. 1976. Multicomponent Mass Transport Model - Theory and Implementation (Discrete Parcel Random Walk Version). BNWL-2127, Battelle Pacific NW Laboratories, Richland. Washington.

PNL. 1976. MMT-DPRW Transport Model User's Guide. Internal document, Battelle Pacific NW Laboratories, Richland, Wash.

Ahlstrom, S.W. and R.G. Baca. 1974. Transport Model User's Manual. BNWL-1716, Battelle Pacific Northwest Laboratories, Richland, Wash.

IGWMC Key: 1950 Model Name: DRAINMOD
Authors: Skaggs, R.W.
Institution of Model Development: North Carolina State University
Dept. of Biological & Agricultural Engineering
Raleigh, North Carolina
Code Custodian: R.W. Skaggs
North Carolina State University
Dept. of Biological and Agric. Eng.
P.O. Box 7625, Raleigh, NC 27695

Abstract:

DRAINMOD is a model for flow and solute transport in shallow, well-drained unsaturated zones. The water balance equation includes terms for gas phase moisture, drainage loss, evapotranspiration loss, outflow to the saturated zone, and infiltration. The model assumes that the soil water content is consistent with fluid

pressure equilibrium conditions. The resulting transient soil water flux rates are used as input into a Petrov-Galerkin advective-dispersive transport model for nonreactive solutes. DRAINMOD solves simultaneously for recharge to the saturated zone, the water table elevation, the equilibrium soil water content distribution, and an evapotranspiration rate, given climatic conditions on an hourly basis as input. The transport module requires solute concentration of recharge water, water content distribution, and velocity profiles at different times.

Model developed for:	research (e.g. hypothesis/theory testing), general use (e.g. in field applications), demonstration/education
Documentation includes:	model theory, user's instructions, example problems, program structure and development, code listing
Verification/validation:	laboratory data sets
Peer (independent) review:	concepts, theory (math)
Availability:	public domain

References:

Skaggs, R.W. 1977. Evaluation of Drainage - Water Table Control Systems Using a Water Management Model. In: Proceed. of the Third National Drainage Symp., ASAE Publication 1-77, pp. 61-68.

Skaggs, R.W. 1978. A Water Management Model for Shallow Water Table Soils. Tech. Rept. No. 134, Water Resources Research Institute of the Univ. of North Carolina, N.C. State Univ., Raleigh, North Carolina.

Skaggs, R.W. 1980. Combination Surface - Subsurface Drainage Systems for Humid Regions. J. Irrigation and Drainage Div. ASCE, Vol. 106(IR4), pp. 265-283.

Skaggs, R.W. and J.W. Gilliam. 1981. Effect of Drainage System Design and Operation on Nitrate Transport. Trans. of the ASAE, Vol. 24(4), pp. 929-934.

Skaggs, R.W., N.R. Fausey and B.H. Nolte. 1981. Water Management Model Evaluation for North Central Ohio. Trans. of the ASAE, Vol. 24(4), pp. 927-928.

Skaggs, R.W., T. Karvonen, and H.M. Kandil. 1991. Predicting Soil Water Flux in Drained Lands. Paper presented at Internat. Summer Meeting, Am. Soc. of Agric. Eng., Albuquerque, New Mexico.

Kandil, H., C.T. Miller, and R.W. Skaggs. 1992. Modeling Long-Term Solute Transport in Drained Unsaturated Zones. Water Resources Res., Vol. 28(10), pp. 2799-2809.

IGWMC Key: 2892 Model Name: GS3

Authors: Davis, L.A., and G. Segol

Institution of Model Development: Water, Waste and Land, Inc.
Fort Collins, Colorado

Code Custodian: Lyle Davis
Water, Waste and Land, Inc.
1311 S. College Avenue
Fort Collins, CO 80524

Abstract:

GS3 is a three-dimensional Galerkin finite element code for analysis of fluid flow and advective-dispersive nonconservative contaminant transport in partially saturated media. The code is particularly useful for simulation of anisotropic systems with strata of varying thickness and continuity. This code contains many of the same features as UNSAT2 (IGWMC Key # 0021) such as the ability to simulate mixed Dirichlet and Neuman boundary conditions for flow and mass transport (concentration of waste leaving the system through evaporated water is zero) by specifying minimum surface pressure and maximum infiltration rate, and seepage faces. However, it will not simulate evapotranspiration by defining a root zone and corresponding plant species data. Unsaturated hydraulic properties are input in table form (no hysteresis).

Model developed for:	research (e.g. hypothesis/theory testing), general use (e.g. in field applications)
Documentation includes:	model theory, user's instructions, example problems, code listing, verification/validation
Verification/validation:	verification (analyt.solutions)
Peer (independent) review:	concepts, theory (math), documentation
Availability:	public domain

References:

Davis, L.A. and G. Segol. 1985. Documentation and User's Guide: GS2 and GS3 - Variably Saturated Flow and Mass Transport Models. NUREG/CR-3901, U.S. Nuclear Regulatory Commission, Washington, D.C.

IGWMC Key: 2891 Model Name: GS2

Authors: Davis, L.A., and G. Segol

Institution of Model Development: Water, Waste and Land, Inc.
Fort Collins, Colorado

Code Custodian: Lyle Davis
Water, Waste and Land, Inc.
1311 S. College Avenue, Fort Collins, CO 80524

Abstract:

GS2 is a two-dimensional Galerkin finite element code for the analysis of flow and contaminant transport in partially saturated media. Either vertical or horizontal plane simulation is possible. The transport equation includes convection, dispersion, radioactive decay, linear equilibrium adsorption and a source/sink term. Boundary conditions for flow may include constant head and constant flux as well as infiltration and evaporation. For transport, boundary conditions may be specified as constant concentration or mass flux. Infiltration and evaporation may occur intermittently. An iterative procedure is used to determine type and length of seepage face boundary.

Model developed for:	research (e.g. hypothesis/theory testing), general use (e.g. in field applications)
Documentation includes:	model theory, user's instructions, example problems, code listing, verification/validation
Verification/validation:	verification (analyt.solutions)
Peer (independent) review:	concepts, theory (math), documentation

References:
Davis, L.A. and G. Segol. 1985. Documentation and User's Guide: GS2 and GS3 - Variably Saturated Flow and Mass Transport Models. NUREG/CR-3901, U.S. Nuclear Regulatory Commission, Washington, D.C..

IGWMC Key: 3377 Model Name: 3DFEMWATER/3DLEWASTE
Authors: Yeh, G.T.
Institution of Model Development: Oak Ridge Nat. Lab. Environm. Sciences Div.
Oak Ridge, Tennessee 37831
Code Custodian: G.T. Yeh
Penn State University, Dept. of Civil Eng.
225 Sackett Bldg, University Park, PA 16802

Abstract:

3DFEMWATER is a three-dimensional finite element model for simulation of water steady state and transient flow through saturated-unsaturated media. The model is designed to handle anisotropic and heterogeneous geologic media, time-varying distributed and point sources and sinks, a wide variety of boundary conditions, including a moving water table and seepage faces. There are three options for estimating the nonlinear matrix, two options for solving the linearized matrix equation, and it includes automatic time step adjustment.

3DLEWASTE is a Langrangian-Eulerian finite element model for simulating advective-dispersive transport of a non-conservative solute. It can be linked with 3DFEMWATER to obtain velocities from flow simulations.

Model developed for:	research (e.g. hypothesis/theory testing), general use (e.g. in field applications)
Documentation includes:	model theory, user's instructions, example problems, program structure and development, code listing, verification/validation
Verification/validation:	verification (analyt.solutions), code intercomparison
Peer (independent) review:	concepts, theory (math), documentation
Availability:	public domain

References:
Yeh, G.T. 1987. 3DFEMWATER: A Three-Dimensional Finite Element Model of Water Flow through Saturated-Unsaturated Media. ORNL-6386. Oak Ridge National Laboratory, Oak Ridge, Tennessee.

IGWMC Key: 3450/3451 Model Name: DISPEQ/DISPER/PISTON
Authors: Fluhler, H., and W.A. Jury
Institution of Model Development: Swiss Federal Inst. of Forest Research
CH 8903 Birmensdorf, Switzerland
Code Custodian: Huber U. Fluhler
240 Nick Davis Road, Madison, AL 35758

Abstract:

DISPEQ/DISPER/PISTON is a series of three finite difference research models to simulate one-dimensional transport of reactive solute species through soil columns, including dispersion, instantaneous equilibrium adsorption (DISPEQ) and rate dependent adsorption (DISPER). PISTON is based on piston type flow without dispersion.

Model developed for: research (e.g. hypothesis/theory testing)
Documentation includes: model theory, user's instructions, example problems, code listing
Verification/validation: laboratory data sets
Availability: public domain

References:

Fluhler, H. and W.A. Jury. 1983. Estimating Solute Transport Using Nonlinear, Rate Dependent, Two-Site Adsorption Models; An Introduction to Use Explicit and Implicit Finite Difference Schemes. Fortran Program Documentation. Rept. 245, Swiss Federal Institution of Forest Research, Birmensdorf, Switzerland.

IGWMC Key: 3540 Model Name: CREAMS
Authors: Knisel, W.G.
Institution of Model Development: USDA Agricultural Research Service
Tuscon, Arizona
Code Custodian: Walter G. Knisel
USDA Agricultural Research Service
Southeast Watershed Research Laboratory
P.O. Box 946, Tifton, GA 31793

Abstract:

CREAMS (A field scale model for Chemicals, Runoff, and Erosion from Agricultural Management Systems) is a general watershed model designed to evaluate non-point source pollution from alternate management practices for field-size areas. It consists of three main components: hydrology, erosion/sedimentation and chemistry. The hydrology model handles storm runoff, infiltration, soil water movement (providing amount of seepage beneath root zone and initial soil water content before a storm), and soil/plant evapotranspiration between storms. The chemistry model includes a nutrient (nitrogen and phosphorus) submodel and a pesticide submodel.

Model developed for: research (e.g. hypothesis/theory testing), general use (e.g. in field applications), demonstration/education
Documentation includes: model theory, user's instructions, example problems, verification/validation
Verification/validation: verification (analyt.solutions)
Availability: public domain

Remarks:

CREAMS was developed for evaluation of agricultural management systems and their effects on non-point pollution potential. CREAMS is the predecessor of GLEAMS (IGWMC Key # 3541).

The USDA Soil Conservation Service released its own version of CREAMS in 1984 (USDA 1984; see references).

References:

Knisel, W.G. (ed.). 1980. CREAMS: A Field Scale Model for Chemicals, Runoff and Erosion from Agricultural Management Systems. Conservation Research Report No. 26, United States Dept. of Agriculture, Tuscon, Arizona.

Knisel, W.G. 1990. CREAMS/GLEAMS: A Development Overview. In: Proceed. of the CREAMS/GLEAMS Symposium, Univ. of Georgia, Athens, Georgia.

U.S. Department of Agriculture. 1984. User's Guide for the CREAMS Model: Washington Computer Center Version. USDA-SCS Engineering Division Technical Release 72. Soil Conservation Service, Washington, D.C.

Laundre, J.W., 1990. Assessment of CREAMS and ERHYP-II Computer Models for Simulating Soil Water Movement on the Idaho National Engineering Laboratory. Radiological and Environmental Sciences Laboratory, U.S. Department of Energy, 46 pp.

IGWMC Key: 4081 Model Name: TRIPM
Authors: Gureghian, A.B.
Institution of Model Development: Office of Nuclear Waste Isolation
Battelle Project Management Div., Columbus, Ohio
Code Custodian: Code custodian
Performance Assessment Dept., Office of Nuclear Waste Isolation,
Battelle Project Management Division
505 King Avenue, Columbus, OH 43201

Abstract:

TRIPM is a two-dimensional finite element model to predict the transport of radionuclides decay chain into and in a phreatic aquifer. It simulates the simultaneous cross-sectional flow water and the transport of reacting solutes through saturated and unsaturated porous media. The influence of soil-water pH on the distribution coefficient is included. Boundary conditions include seepage faces.

Model developed for:	research (e.g. hypothesis/theory testing), general use (e.g. in field applications)
Documentation includes:	model theory, user's instructions, example problems, program structure and development, code listing, verification/validation
Verification/validation:	verification (analyt.solutions)
Peer (independent) review:	concepts, theory (math), coding, documentation
Availability:	public domain

References:

Gureghian, A.B. 1983. TRIPM: A Two-Dimensional Finite Element Model for the Simultaneous Transport of Water and Reacting Solutes through Saturated and Unsaturated Porous Media. ONWI-465, Off. of Nuclear Waste Isolation, Battelle Project Management Div., Columbus, Ohio.

Gureghian, A.B. 1981. A Two-Dimensional Finite-Element Solution Scheme for the Saturated-Unsaturated Flow with Applications to Flow through Ditch-Drained Soils. Journ. of Hydrology, Vol. 50, pp. 1-20.

IGWMC Key: 4270 Model Name: TRACR3D
Authors: Travis, B.J.
Institution of Model Development: Los Alamos National Laboratory
Los Alamos, New Mexico
Code Custodian: Travis, B.J.
Los Alamos National Laboratory, MS-F665
Los Alamos, NM 87545

Abstract:

TRACR3D is a three-dimensional implicit (for flow)/semi-implicit (for transport) finite difference model for simulation of transient two-phase flow of water and air, and of non-conservative multi-component transport in deformable, heterogeneous, water-saturated or variably-saturated, reactive porous and/or fractured media. Flow of liquid and gas is coupled using Brooks and Corey expressions for relative hydraulic conductivity of liquid and gas. Transport processes include advection, dispersion, sorption, and decay. The model can handle simple steady-state, one-dimensional, single phase problems to complex, transient, two-phase flow and tracer transport.

Model developed for:	research (e.g. hypothesis/theory testing), general use (e.g. in field applications)
Documentation includes:	model theory, user's instructions, example problems, program structure and development, code listing, verification/validation
Verification/validation:	verification (analyt.solutions), laboratory data sets
Peer (independent) review:	concepts, theory (math)
Availability:	public domain

References:

Travis, B. 1984. TRACR3D: A Model of Flow and Transport in Porous/Fractured Media. Los Alamos National Lab., Report LA-9667-MS, Los Alamos, New Mexico.

IGWMC Key: 4290 Model Name: CADIL/AGTEHM

Authors: Emerson, C.J., B. Thomas, R.J. Luxmoore, and D.M. Hetrick

Institution of Model Development: Oak Ridge National Laboratory
Oak Ridge, Tennessee

Code Custodian: Emerson, C.J.
Oak Ridge National Laboratory, Computer Sciences Department
Oak Ridge, TN 37831

Abstract:

CADIL (Chemical Adsorption and Degradation In Land) is a moisture and chemical species mass balance model which simulates chemical transport through soils. It includes the processes of deposition, infiltration, adsorption (Freundlich isotherm) and first-order (bio-)chemical degradation of chemicals. It also simulates the effect of soil temperature on chemical degradation. Chemical transport in soil water may be either vertical or lateral. Both macropore and matrix flows of chemicals in soil water are modeled. CADIL couples to AGTEHM, which in turn calculates soil water transport through the bulk matrix and soil macro-pores. AGTEHM simulates interception, throughfall, infiltration, soil evaporation, plant transpiration, and surface runoff.

Model developed for:	research (e.g. hypothesis/theory testing), general use (e.g. in field applications)
Documentation includes:	model theory, user's instructions, example problems. program structure and development, code listing, verification/validation
Verification/validation:	verification (analyt.solutions)
Peer (independent) review:	concepts, theory (math)
Availability:	public domain

Remarks:

The CADIL model is executed as a submodel of the AGTEHM model (Hetrick et al. 1982; see references; see also IGWMC Key # 3390). It was developed from SCEHM, an earlier soil chemical model developed by Begovich and Jackson (1975; see references.)

References:

Emerson, C.J.; B. Thomas, Jr. and R.J. Luxmoore. 1984. CADIL: Model Documentation for Chemical Adsorption and Degradation in Land. ORNL/TM-8972, Oak Ridge National Lab., Oak Ridge, Tennessee.

Begovich, C.L. and D.R. Jackson. 1975. Documentation and Application of SCEHM - A Model for Soil Chemical Exchange of Heavy Metals. ORNL/NSF/EATC-16, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

Hetrick, D.M., J.T. Holdeman, and R.J. Luxmoore. 1982. AGTEHM: Documentation of Modifications to the Terrestrial Ecosystem Hydrology Model (TEHM) for Agricultural Applications. ORNL/TM-7856, Oak Ridge National Lab., Oak Ridge, Tennessee.

Huff, D.D., R.J. Luxmoore, J.B. Mankin, and C.L. Begovich. 1977. TEHM: A Terrestrial Ecosystem Hydrology Model. ORNL/NSF/EATC-27, Oak Ridge National Lab., Oak Ridge, Tennessee.

IGWMC Key: 4391 Model Name: SBIR

Authors: Li, R-M.

Institution of Model Development: U.S. Bureau of Reclamation
Washington, D.C.

Code Custodian: Li, Ruh-Ming
3901 Westerly Place, Suite 101
Newport Beach, CA 92660

Abstract:

SBIR is a three-dimensional finite difference model for simulation of flow and mass transport in a variable saturated porous medium. A vector processor is used in the solution. Benchmark tests indicated the relatively high efficiency of the code.

Model developed for: research (e.g. hypothesis/theory testing)

Documentation includes: model theory, user's instructions, example problems, program structure and development, code listing, verification/validation

Verification/validation: verification (analyt.solutions)

References:

Bureau of Reclamation. 1987. SBIR Phase I Final Report. Modeling Physics and Chemistry of Contaminant Transport in Three-Dimensional Unsaturated Ground-Water Flow. Final Rept. Contract 4-CR-93-00010. U.S. Dept. of the Interior, Washington, D.C. (NTIS access # PB85-160683).

Li, R-M, K.G. Eggert and K. Zachmann. 1983. Parallel Processor Algorithm for Solving Three-Dimensional Ground Water Flow Equations. National Science Foundation, Washington, D.C.

IGWMC Key: 4570 Model Name: VS2D/VS2DT

Authors: Lappala, E.G., R.W. Healy, and E.P. Weeks
Institution of Model Development: U.S. Geological Survey
Denver Federal Center, Lakewood, Colorado
Code Custodian: Weeks, E.P.
U.S. Geological Survey
Box 25046, M.S. 413, Denver Federal Center,
Denver, CO 80225

Abstract:

VS2D is a two-dimensional finite difference simulator for cross-sectional or cylindrical variably saturated flow in porous media. The model allows consideration of non-linear storage, conductance, and sink terms and boundary conditions. Processes included are infiltration, evaporation and plant root uptake. The program also handles seepage faces. VS2DT is a solute transport module to be used with VS2D. It is based on a finite difference approximation of the advection-dispersion equation for a single species. Program options include first-order decay, equilibrium adsorption described by Freundlich or Langmuir isotherms, and ion-exchange. Nonlinear storage terms are linearized by an implicit Newton-Raphson method. (see also remarks).

Nonlinear conductance terms, boundary conditions, and sink terms are linearized implicitly. Relative hydraulic conductivity is evaluated at cell boundaries by using full upstream weighing, the arithmetic mean, or the geometric mean of values of adjacent cells. Saturated hydraulic conductivities are evaluated at cell boundaries by using distance weighted harmonic means. The linearized matrix equations are solved using the strongly implicit method. Nonlinear conductance and storage coefficients are represented by closed-form algebraic equations or interpolated from tables.

Nonlinear boundary conditions treated by the code include infiltration, evaporation, and seepage faces. Extraction by plant roots is included as a nonlinear sink term.

Initial conditions may be input as moisture content or pressure head by blocks defined by row and column, or in a formatted file by cell. An equilibrium profile may be specified above a user defined free water surface. Infiltration may be simulated by specified flux nodes, specified pressure nodes, or a ponding function where the user specifies rainfall rate and ponding height. Evaporation is simulated by a user defined potential evapotranspiration, pressure potential of the atmosphere, and surface resistance. Evapotranspiration is simulated through the use of user defined potential evapotranspiration, minimum root pressure, depth of rooting, and root activity at the bottom of the root zone and land surface. Seepage faces may also be simulated

Model developed for:	research (e.g. hypothesis/theory testing), general use (e.g. in field applications)
Documentation includes:	model theory, user's instructions, example problems, program structure and development, code listing, verification/validation
Verification/validation:	verification (analyt.solutions)
Peer (independent) review:	concepts, theory (math), documentation
Availability:	public domain, proprietary, purchase

Remarks:

A PC version is available from the International Ground Water Modeling Center (Colorado School of Mines, Golden, CO 80401), which includes a user interface for data entry and program execution. It requires Intel 80386 based microcomputer with at least 4M bytes RAM and a math co-processor.

The computer program VS2D, which simulates water movement through variably saturated porous media, was published in 1987 (Lappala et Al. 1987; see references). The computer program VS2DT, which includes both non-linear water flow and solute transport, was released in 1990. It included a slightly modified version of VS2D (Healy 1990; see references).

References:

Lappala, E.G., R.W. Healy and E.P. Weeks, 1987. Documentation of Computer Program VS2D to Solve the Equations of Fluid Flow in Variably Saturated Porous Media. Water Resources Investigations Report 83-4099. U.S. Geological Survey, Denver, Colorado.

Healy, R.W. 1987. Simulation of Trickle Irrigation, an Extension to the U.S. Geological Survey's Computer Program VS2D. Water Resources Investigations Report 87-4086, U.S Geological Survey, Denver, Colorado.

Healy, R.W. 1990. Simulation of Solute Transport in Variably Saturated Porous Media with Supplemental Information on Modifications to the U.S. Geological Survey's Computer Program VS2D. Water-Resources Investigations Report 90-4025, U.S. Geological Survey, Denver, Colorado.

IGWMC Key: 4630 Model Name: FLAMINCO

Authors: Huyakorn, P.S.
Institution of Model Development: GeoTrans, Inc
Sterling, Virginia
Code Custodian: David Ward
GeoTrans, Inc.
46050 Manekin Plaza, Suite 100, Sterling, VA 22170

Abstract:

FLAMINCO is a three-dimensional upstream weighted finite element model to simulate transient water flow and solute transport processes in fully- and variably saturated porous media. Transport processes included are advection, hydrodynamic dispersion, linear equilibrium adsorption and first-order decay. Nonlinearities due to unsaturated soil properties and atmospheric boundary conditions are treated using Picard iterations. The model uses a Slice Successive Over Relaxation (SSOR) matrix solution scheme.

Model developed for:	general use (e.g. in field applications)
Documentation includes:	model theory, user's instructions, example problems, program structure and development, verification/validation
Verification/validation:	verification (analyt.solutions), laboratory data sets
Peer (independent) review:	concepts, theory (math)
Availability:	proprietary, license

References:

Huyakorn, P.S. and T.D. Wadsworth. 1985. FLAMINCO: A Three-Dimensional Finite Element Code for Analyzing Water Flow and Solute Transport in Saturated-Unsaturated Porous Media. Techn. Rept. for U.S. Dept. of Agriculture, Northwest Watershed Research Center, Boise, Idaho, Contract Nr. 53-3K06-4-82, GeoTrans, Inc., Sterling, Virginia.

Huyakorn, P.S., E.P. Springer, V. Guvanasen, and T.D. Wadsworth. 1986. A Three-Dimensional Finite Element Model for Simulation of Solute Transport in Variably-Saturated Porous Media. Water Resources Research, Vol. 22(13), pp. 1790-1808.

IGWMC Key: 5039 Model Name: SESOIL (Seasonal Soil Compartment Model)

Authors: Bonazountas, M.
Institution of Model Development: Arthur D. Little
Boston, Massachusetts
Code Custodian: David Hetrick
8417 Mecklenburg Court, Knoxville, TN 37923

Abstract:

SESOIL is a user-friendly finite-difference soil compartment model designed for long-term hydrologic, sediment, and pollutant fate simulations. The model distinguishes three major components, the hydrological cycle, the sediment cycle and pollutant transport and fate. Elements of the hydrologic cycle included are rainfall, soil moisture variations, infiltration, exfiltration, surface runoff, evapotranspiration, and groundwater runoff; simulation of the sediment cycle include sediment washload from storms and sediment resuspension due to wind; the pollutant fate cycle simulated takes into account advection, diffusion, volatilization, adsorption and desorption, chemical degradation or decay, biological transformations, hydrolysis, complexation, and ion exchange.

Model developed for:	research (e.g. hypothesis/theory testing), general use (e.g. in field applications)
Documentation includes:	model theory, user's instructions, example problems, verification/validation
Verification/validation:	verification (analyt.solutions)
Peer (independent) review:	concepts, theory (math)
Availability:	public domain; some versions are proprietary

Remarks:

SESOIL has undergone testing by a variety of organizations. These efforts have included sensitivity analysis, comparison with other models, and limited comparison with field data (Bonazountas et Al, 1982; Wagner et Al., 1983; Hetrick, 1984; Hetrick et Al., 1982, 1986; Bicknell et Al., 1984; Kincaid et Al., 1984; Watson and Brown, 1985; Donigian and Rao, 1986; and Hetrick et Al. 1988a, 1988b; see references).

SESOIL was incorporated as the soil/land component of the screening level multimedia model, TOX-SCREEN (Hetrick and McDonald-Boyer, 1984), developed by Oak Ridge National Laboratory, Oak Ridge, Tennessee for EPA's Office of Toxic Substances.

The comprehensive evaluation of SESOIL by Watson and Brown (1985) uncovered numerous deficiencies in the original version of the model. Subsequently, SESOIL has been extensively modified at Oak Ridge National Laboratory to enhance its capabilities. This modified version is incorporated in the Graphical Exposure Modeling System developed for EPA/OTS (GEMS; see Kinerson and Hall, 1986). This version will be available from the International Ground Water Modeling Center, Fall 1992.

References:

Bonazountas, M., J. Wagner, and B. Goodwin. 1982. Evaluation of Seasonal Soil/Groundwater Pollutant Pathways. Arthur D. Little, Inc., Cambridge, Mass.

Wagner, J., M. Bonazountas, and M. Alsterberg. 1983. Potential Fate of Buried Halogenated Solvents via SESOIL. Arthur D. Little, Inc., Cambridge, Mass.

Hetrick, D.M. 1984. Simulation of the Hydrologic Cycle for Watersheds. In: Proceedings of the 9th IASTED International Conference, San Francisco, Calif.

Hetrick, D.M., J.T. Holdeman, and R.J. Luxmore. 1982. AGTHEM: Documentation of Modifications to the Terrestrial Ecosystem Model (THEM) for Agricultural Applications. ORNL/TM-7856, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

Hetrick, D.M., and L.M. McDonald-Boyer. 1984. User's Manual for TOX-SCREEN: Multimedia Screening-Level Program for Assessing Potential Fate of Chemicals Released to the Environment. ORNL-6041, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

Bicknell, B.R., S.H. Boutwell, and D.B. Watson. 1984. Testing and Evaluation of the TOX-SCREEN Model. Anderson-Nichols and Co., Palo Alto, Calif.

Kincaid, C.T., J.R. Morey, S.B. Yabusaki, A.R. Felmy, and J.E. Rogers. 1984. Geohydrochemical Models for Solute Migration, Volume 2: Preliminary Evaluation of Selected Computer Codes for Modeling Aqueous Solutions and Solute Migration in Soils and Geologic Media. EA-3417, Electric Power Research Instit., Palo Alto, Calif.

Watson, D.B., and S.M. Brown. 1985. Testing and Evaluation of the SESOIL Model. Anderson-Nichols and Co., Palo Alto, Calif.

Bonazountas, M. and J.M. Wagner. 1984. "SESOIL" A Seasonal Soil Compartment Model. EPA Contract No. 68-01-6271, by Arthur D. Little, Cambridge, Mass. for U.S. Environmental Protection Agency, Office of Toxic Substances, Washington, D.C.

Donigian, Jr., A.S., and P.S.C. Rao. 1986. Overview of Terrestrial Processes and Modeling. In: S.C. Hern and S.M. Melancon (eds.), Vadose Zone Modeling of Organic Polllutants. Lewis Publishers, Chelsea, Michigan.

Hetrick, D.M., C.C. Travis, P.S. Shirley, and E.L. Etnier. 1986. Model Predictions of Watershed Hydrologic Components: Comparison and Verification. Water Resourc. Bull., Vol. 22(5), pp. 803-810.

Hetrick, D.M., C.C. Travis, S.K. Leonard, and R.S. Kinerson. 1988a. Qualitative Validation of Pollutant Transport Components of an Unsaturated Soil Zone Model (SESOIL). ORNL/TM-10672, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

Hetrick, D.M., C.C. Travis, and R.S. Kinerson. 1988b. Comparison of an Unsaturated Soil Zone Model (SESOIL) Predictions with a Laboratory Leaching Experiment. CONF-881209--1, Oak Ridge National Lab., Oak Ridge, Tennessee.

Kinerson, R.S., and L. Hall. 1986. Graphical Exposure Modeling System (GEMS) User's Guide. Office of Toxic Substances, U.S. Environmental Protection Agency, Washington, D.C.

IGWMC Key: 4690 Model Name: VAM2D (Variably saturated Analysis Model in 2 Dimensions)
Authors: Huyakorn, P.S.
Institution of Model Development: HydroGeologic, Inc., Herndon, Virginia

Code Custodian: Jan Kool, HydroGeologic, Inc.
1165 Herndon Parkway, Suite 100, Herndon, VA 22070

Abstract:

VAM2D is a two-dimensional Galerkin finite element model to simulate flow and contaminant transport in variably saturated porous media. The code can perform simulations in an areal plane, a cross-section, or an axisymmetric configuration. The highly nonlinear soil moisture relations can be treated using Picard or Newton-Raphson iterations. The model uses the upstream weighted residual method to treat the advective-dispersive transport equation with linear or non-linear equilibrium sorption, and first-order degradation. Cross-sectional unconfined flow problems can be analyzed using a rigorous unsaturated-saturated modeling approach or an approximate saturated-pseudo unsaturated modeling approach that does not require user-supplied soil moisture relations.

Model developed for: general use (e.g. in field applications)
Documentation includes: model theory, user's instructions, example problems, verification/validation
Verification/validation: verification (analyt.solutions), code intercomparison
Peer (independent) review: concepts, theory (math)
Availability: proprietary, license

Remarks:

The model VAM2D is a descendant of the formulation used in the SATURN code presented by Huyakorn et Al (1984, 1985; see references). The VAM2D code has been checked by its authors against available analytical or semi-analytical solutions and similar numerical codes including UNSAT2, FEMWATER/FEMWASTE, and SATURN.

References:

Huyakorn, P.S., J.W. Mercer and D.S. Ward. 1985. Finite Element Matrix and Mass Balance Computational Schemes for Transport in Variably Saturated Porous Media. Water Resources Research, Vol. 21(3), pp. 346-358.

Huyakorn, P.S. and S.D. Thomas. 1984. Techniques for Making Finite Elements Competitive in Modeling Flow in Variably Saturated Porous Media. Water Resourc. Res., Vol. 20(8), pp. 1099-1115.

Huyakorn, P.S., et Al. 1987. Finite Element Simulation of Moisture Movement and Solute Transport in a Large Caisson. In: Modeling Study of Solute Transport in the Unsaturated Zone, NUREG/CR 4515-2, pp. 117-170. U.S. Nuclear Regulatory Commission, Washington, D.C.

IGWMC Key: 4691 Model Name: VAM3D
Authors: Huyakorn, P.S.
Institution of Model Development: HydroGeologic, Inc., Herndon, Virginia

Code Custodian: Jan Kool, HydroGeologic, Inc.
1165 Herndon Parkway, Suite 100, Herndon, VA 22070

Abstract:

VAM3D (Variably saturated Analysis Model in 3 Dimensions) is a three-dimensional finite-element model for simulation of flow and contaminant transport in variably saturated porous media. It is capable of steady-state and transient simulations in an areal plane, a cross-section, an axisymmetric configuration, or a fully three-dimensional mode using rectangular and triangular prisms. Nonlinearities in the unsaturated flow equation is solved using Picard iteration. The matrix equations are solved using a slice-successive over-relaxation scheme or conjugate gradient algorithms. The advective-dispersive transport equation is solved using upstream weighted procedure. Transport includes linear and Freundlich adsorption isotherms and first-order degradation. An element mesh generator is available.

Model developed for:	general use (e.g. in field applications)
Documentation includes:	model theory, user's instructions, example problems, verification/validation
Verification/validation:	verification (analyt.solutions), code intercomparison
Peer (independent) review:	concepts, theory (math)
Availability:	proprietary, license

Remarks:

The formulation used in VAM3D is a descendent of the formulation used in the FLAMINCO code presented by Huyakorn et Al. (1986; see references). Where possible, VAM3D has been checked by its authors against available analytical or semi-analytical solutions and similar numerical codes including UNSAT2, FEMWATER/FEMWAST, SATURN and FLAMINCO.

References:

Huyakorn, P.S., E.P. Springer, V. Guvanasen, and T.D. Wadsworth. 1986. A Three-Dimensional Finite Element Model for Simulation of Solute Transport in Variably-Saturated Porous Media. Water Resources Research, Vol. 22(13), pp. 1790-1808.

Huyakorn, P.S., et Al. 1987. Finite Element Simulation of Moisture Movement and Solute Transport in a Large Caisson. In: Modeling Study of Solute Transport in the Unsaturated Zone, NUREG/CR 4515-2, pp. 117-170. U.S. Nuclear Regulatory Commission, Washington, D.C.

Huyakorn, P.S., J.W. Mercer and D.S. Ward. 1985. Finite Element Matrix and Mass Balance Computational Schemes for Transport in Variably Saturated Porous Media. Water Resources Research, Vol. 21(3), pp. 346-358.

IGWMC Key: 4720 Model Name: PRZM

Authors: Carsel, R.F., C.N. Smith, L.A. Mulkey, and J.D. Dean

Institution of Model Development: U.S. Environmental Protection Agency
Environmental Research Lab., Athens, Georgia

Code Custodian: R.F. Carsel
U.S. Environmental Protection Agency
Environmental Research Lab., Athens, GA 30613

Abstract:

PRZM (Pesticide Root Zone Model) simulates the vertical movement of pesticides in the unsaturated zone within and below the root zone. The model consists of hydrologic and chemical transport components to simulate runoff, erosion, plant uptake, leaching, decay, foliar washoff, and volatilization. Pesticide transport and fate processes include advection, dispersion, molecular diffusion, and soil sorption. Predictions can be made for daily, monthly or annual output. A finite difference numerical solution, using a backwards difference

implicit scheme, is employed. PRZM allows the user to perform dynamic simulations considering pulse loads, predicting peak events, and estimating time-varying emission or concentration profiles in layered soils. (see also remarks).

Model developed for:	research (e.g. hypothesis/theory testing), general use (e.g. in field applications), demonstration/education
Documentation includes:	model theory, user's instructions, example problems, verification/validation
Verification/validation:	verification (analyt.solutions), laboratory data sets
Peer (independent) review:	concepts, theory (math), documentation
Availability:	public domain

Remarks:

PRZM is a one-dimensional finite difference model which accounts for pesticide fate and transport in the crop root zone. It includes soil temperature effects, volatilization and vapor phase transport in soils, irrigation simulation and a method of characteristics algorithm to eliminate numerical dispersion. PRZM is capable of simulating fate and transport of the parent and up to two daughter species.

PRZM, VADOFT and SAFTMOD are part of RUSTIC. RUSTIC (MARS Key # 4721) links these models in order to predict the fate and transport of chemicals to drinking water wells. The codes are linked together with the aid of a flexible execution supervisor (software user interface) that allows the user to build models that fit site-specific situations.

Wagner and Ruiz (1986; see IGWMC Key # 5310) designed an aquifer linkage model PRZMAL to connect PRZM with the analytical three-dimensional model PLUME 3D.

References:

Carsel, R.F., C.N. Smith, L.A. Mulkey, J.D. Dean, and P. Jowise. 1984. User's Manual for the Pesticide Root Zone Model (PRZM), Release 1. EPA-600/3-84-109, U.S. Environmental Protection Agency, Environmental Research Lab., Athens, Georgia.

Carsel, R.F., L.A. Mulkey, M.N. Lorber, and L.B. Baskin. 1985. The Pesticide Root Zone Model (PRZM): A Procedure for Evaluating Pesticide Leaching Threats to Ground Water. Ecological Modeling, Vol. 30, pp. 49-69.

Donigian, Jr., A.S., and P.S.C. Rao. 1986. Overview of Terrestrial Processes and Modeling. In: S.C. Hern and S.M. Melancon (eds.), Vadose Zone Modeling of Organic Polllutants. Lewis Publishers, Chelsea, Michigan.

IGWMC Key: 6620 Model Name: RITZ

Authors: Nofziger, D.L. (1) , J.R. Williams (2), and T.E. Short (2)

Institution of Model Development: 1) Oklahoma State University, Stillwater, Oklahoma
2) U.S. EPA, R.S. Kerr Env. Res. Lab., Ada, Oklahoma

Code Custodian: J.R. Williams
Robert S. Kerr Environm. Research Lab.
U.S. Environmental Protection Agency
P.O. Box 1198, Ada, OK 74820

Abstract:

RITZ (Regulatory and Investigative Treatment Zone model) is an interactive program for simulation of the movement and fate of hazardous chemicals during land treatment of oily wastes. The model considers a constant water flux and downward movement of the pollutant with the soil solution (leaching), volatilization and loss to the atmosphere, and (bio-)chemical degradation. The treatment site modeled consists of a plow zone and a treatment zone. The model incorporates the influence of oil upon the transport and fate of the pollutant. As input the model requires the properties of the chemicals and oil in the waste material, the soil properties of the treatment site, the management practices, and the parameters relevant to the environment of the site.

Model developed for:	research (e.g. hypothesis/theory testing), general use (e.g. in field applications), demonstration/education
Documentation includes:	model theory, user's instructions, example problems, verification/validation
Verification/validation:	verification (analyt.solutions), laboratory data sets, field datasets (validation)
Peer (independent) review:	concepts, theory (math), documentation
Availability:	public domain

References:

Nofziger, D.L., J.R. Williams, and T.E. Short. 1988. Interactive Simulation of the Fate of Hazardous Chemicals During Land Treatment of Oily Wastes: RITZ User's Guide. EPA/600/8-88/001, R.S. Kerr Env. Research Lab., U.S. Env. Protection Agency, Ada, Oklahoma.

Short, T.E. 1988. Movement of Contaminants from Oily Wastes During Land Treatment. In: Soils Contaminated by Petroleum: Environmental and Public Health Effects. Proceedings Conf. on Environm. and Public Health Effects of Petroleum Contaminated Soils, Univ. of Mass., Amherst, Mass. Oct. 30-31, 1985.

IGWMC Key: 6640 Model Name: CHEMRANK

Authors: Nofziger, D.L., P.S.C. Rao, and A.G. Hornsby

Institution of Model Development: Institute of Food and Agricultural Sciences
University of Florida, Gainesville, Florida

Code Custodian: Institute of Food and Agricultural Sciences
University of Florida, Gainesville, FL 32611

Abstract:

CHEMRANK is an interactive package which utilizes four ranking schemes for screening organic chemicals relative to their potential to leach into groundwater systems. The schemes are based on rates of chemical movement or relative rates of mobility and degradation of the chemicals within the vadose zone. Two schemes use steady state groundwater recharge rates and the other two require daily rainfall and evaporation data. The latter two schemes rank chemical mobility by travel time in the vadose zone or mass emission of selected chemicals at some specified depth in the vadose zone.

Model developed for:	research (e.g. hypothesis/theory testing), general use (e.g. in field applications), demonstration/education
Documentation includes:	model theory, user's instructions, example problems
Availability:	public domain

References:

Nofziger, D.L., P.S.C. Rao, and A.G. Hornsby. 1988. CHEMRANK: Interactive Software for Ranking the Potential of Organic Chemicals to Contaminate Groundwater. Inst. of Food and Agric. Sciences, University of Florida, Gainesville, Florida.

IGWMC Key: 5021 Model Name: BIOSOIL

Authors: Baek, N.H.

Institution of Model Development: Rensselaer Polytechnic Institute
Dept. of Environmental Eng.
Troy, New York 12181

Code Custodian: N.H. Baek
Occidental Chemical Corporation, Technology Center
2801 Long Road, Grand Island, NY 14072

Abstract:

The system modeled by BIOSOIL consists of four components: 1) soil water flow to transport a limiting substrate and a recalcitrant chemical; 2) chemical persistence mitigated by an ultimate removal mechanism of biodegradation; 3) soil microbial growth enriched by exogenous supply of a limiting substrate; and 4) substrate availability to support soil microbial growth for the enhancement of chemical removal. Variable-step and variable order Gear's method is employed as a numerical approximation to solve the set of four ODE's which result from the transformation of four PDE's via the finite difference method. The response of the system to different values for such model inputs as substrate concentration, application rate, and application cycle can be studied.

Model developed for: research (e.g. hypothesis/theory testing)
Documentation includes: model theory, user's instructions, example problems, code listing
Peer (independent) review: concepts, theory (math)
Availability: public domain

References:

Baek, N.H. 1986. A Mathematical Model (BIOSOIL) for the Mitigation of Chemical Persistence by Microbial Enrichment in the Unsaturated Zone. Ph.D. Thesis, Rensselaer Polytechnic Institute, Troy, New York.

IGWMC Key: 5028 Model Name: GTC (Group Transfer Concentration)

Authors: Yu, C., W.A. Jester, and A.R. Jarrett

Institution of Model Development: Argonne National Laboratory
Argonne, IL 60439

Code Custodian: Charles Yu
Argonne National Laboratory, 9700 S. Cass Avenue, Argonne, IL 60439

Abstract:

GTC is a general purpose finite difference solute transport model developed to simulate solute movement in heterogeneous porous media. It splits up the modeled area in zones of constant properties, including dispersion coefficient, retardation factor, and degradation rate. Mass transfer between the solid phase and the liquid phase is proportional to the concentration gradient. The GTC model can be used for both saturated and unsaturated conditions. It covers the conventional advection-dispersion model, the mobile-immobile pore model, the nonequilibrium adsorption-desorption model and the jointed porous rock model.

Model developed for: research (e.g. hypothesis/theory testing), general use (e.g. in field applications)
Documentation includes: model theory
Availability: restricted public domain

References:

Yu, C., W.A. Jester, and A.R. Jarrett. 1985. A General Solute Transport Model and its Applications in Contaminant Migration Analysis. CONF-850893--1, Argonne National Lab., Argonne, Illinois.

IGWMC Key: 6710 Model Name: CMIS (Chemical Movement in Soil)
Authors: Nofziger, D.L., and A.G. Hornsby
Institution of Model Development: Florida Coop. Extension Service
University of Florida, Gainesville, Florida
Code Custodian: Inst. of Food and Agric. Sciences, IFAS
University of Florida, Building 664, Gainesville, FL 32611

Abstract:

CMIS is a management/educational computer program that provides qualitative predictions of pesticide fate as function of key soil, chemical, and climatic variables. Model assumptions limit it to nonpolar pesticides (and other xenobiotics) moving in sandy soils. Linear adsorption/desorption isotherms are used to describe chemical affinity to the soil matrix.

Model developed for: research (e.g. hypothesis/theory testing), general use (e.g. in field applications), demonstration/education
Documentation includes: model theory, user's instructions, example problems, verification/validation
Verification/validation: verification (analyt.solutions), laboratory data sets
Peer (independent) review: concepts, theory (math)
Availability: proprietary, purchase

Remarks:

An updated and expanded version of CMIS by the same author is CMLS (Chemical Movement in Layered Soils); Nofziger and Hornsby, 1988 (see references); also IGWMC Key # 6711.

References:

Nofziger, D.L., and A.G. Hornsby. 1985. Chemical Movement in Soils: IBM PC User's Guide. Circular 654, Florida Coop. Ext. Serv., Univ. of Florida, Gainesville, Florida.

O'Connor, G.A., and F. Khorsandi. 1986. Predicting Chemical Movement in Soils. WRRI Rept. M17, New Mexico Water Resources Research Inst., New Mexico State Univ., Las Cruces, New Mexico.

Nofziger, D.L., and A.G. Hornsby. 1988. Chemical Movement in Layered Soils: User's Manual. Circular 780, Inst. of Food and Agric. Sciences, Univ. of Florida, Gainesville, Florida. (Also: Computer Software Series CCS-30, Agric. Exp. Station, Div. of Agric., Oklahoma State Univ., Stillwater, Oklahoma).

Nofziger, D.L., R.S. Mansell, L.B. Baldwin, and M.F. Laurent. 1983. Pesticides and their Behavior in Soil and Water. Report SL-40 (revised), Florida Cooperative Extension Service, University of Florida, Gainesville, Florida.

IGWMC Key: 6711 Model Name: CMLS (Chemical Movement in Layered Soils)
Authors: Nofziger, D.L. (1), and A.G. Hornsby (2)
Institution of Model Development: 1) Oklahoma State University, Stillwater, Oklahoma
2) University of Florida, Gainesville Florida
Code Custodian: Inst. of Food and Agric. Sciences, IFAS
University of Florida, Building 664, Gainesville, FL 32611

Abstract:

CMLS is an interactive microcomputer model to be used as management tool and a decision aid in the application of organic chemicals to soils. The model estimates the location of the peak concentration of non-polar organic chemicals as they move through a soil in response to the downward movement of water. The model also estimates the relative amount of each chemical still in the soil at any time. The model can deal with soils with up to 20 layers or horizons, each having its own partition coefficient and degradation half-life of the chemical of interest.

Model developed for:	research (e.g. hypothesis/theory testing), general use (e.g. in field applications), demonstration/education
Documentation includes:	model theory, user's instructions, example problems, verification/validation
Verification/validation:	verification (analyt.solutions)
Peer (independent) review:	concepts, theory (math)
Availability:	proprietary, purchase

Remarks:

This software is based on a model published by Nofziger and Hornsby (1986; see references). That model is an expansion of the model presented by Rao et Al (1976; see references). It is also an expansion of the CMIS (Chemical Movement in Soils) model of Nofziger and Hornsby (1985; see IGWMC Key # 6710).

References:

Nofziger, D.L., and A.G. Hornsby. 1988. Chemical Movement in Layered Soils: User's Manual. Circular 780, Inst. of Food and Agric. Sciences, Univ. of Florida, Gainesville, Florida. (Also: Computer Software Series CCS-30, Agric. Exp. Station, Div. of Agric., Oklahoma State Univ., Stillwater, Oklahoma).

Nofziger, D.L., and A.G. Hornsby. 1986. A Microcomputer-Based Management Tool for Chemical Movement in Soil. Applied Agric. Research, Vol. 1, pp. 50-56.

Rao, P.S.C., J.M. Davidson, and L.C. Hammond. 1976. Estimation of Nonreactive and Reactive Solute Front Locations in Soils. EPA-600/9-075-015, Office of Research and Developm, U.S. Env. Protection Agency, Washington, D.C.

IGWMC Key: 3541 Model Name: GLEAMS
Authors: Leonard, R.A., W.G. Knisel, and F.M. Davis
Institution of Model Development: U.S.D.A. Agricultural Research Station
Southeast Watershed Experimental Station
Tifton, Georgia
Code Custodian: R.A. Leonard, W.G. Knisel or F.M. Davis
USDA-ARS, P.O. Box 946, Tifton, GA 31793

Abstract:

GLEAMS (Groundwater Loading Effects on Agricultural Management Systems) was developed as an extension of an earlier USDA model, CREAMS. Both models simulate soil water balance and surface transport of sediments and chemicals from agricultural field management units. GLEAMS, in addition, simulates chemical transport in and through the plant root zone. Several other features were added such as irrigation/chemigation options, pesticide metabolite tracking, and software to facilitate model implementation and output data analysis. Input requirements for the model include daily rainfall volumes, crop and management parameters; soil and physical parameters; pesticide property data such as solubility, and expected half-life in soil and/or foliage.

Model developed for:	research (e.g. hypothesis/theory testing), general use (e.g. in field applications), demonstration/education
Documentation includes:	model theory, user's instructions, example problems, program structure and development, code listing, verification/validation
Verification/validation:	laboratory data sets, field datasets (validation)
Availability:	public domain

Remarks:

As of mid 1990, since its release in late 1986, over 500 copies of GLEAMS have been provided to users worldwide (Leonard et al. 1990). Since its first release it has been constantly updated and expanded.

The predecessor to GLEAMS, CREAMS, is annotated as IGWMC key # 3540.

References:

Leonard, R.A., W.G. Knisel, and D.A. Still. 1987. GLEAMS: Groundwater Loading Effects of Agricultural Management Systems. Transactions of ASEA, Vol. 30(5), pp. 1403-1418.

Knisel, W.G. 1990. CREAMS/GLEAMS: A Development Overview. In: Proceed. of the CREAMS/GLEAMS Symposium, Univ. of Georgia, Athens, Georgia.

Leonard, R.A., W.G. Knisel, F.M. Davis, and A.W. Johnson. 1988. Modeling Pesticide Metabolite Transport with GLEAMS. In: Proceed. ASCE, Irrigation and Drainage Specialty Conference, Lincoln, Nebraska, July 11-14, pp. 255-262. Am. Soc. of Civil Eng., Boston, Mass.

Leonard, R.A., W.G. Knisel, F.M. Davis, and A.W. Johnson. 1990. Validating GLEAMS with Field Data for Fenamiphos and its Metabolites. Journ. Irrigation and Drainage Eng., Vol. 116, pp. 24-35.

Leonard, R.A., W.G. Knisel, and F.M. Davis. 1990. The GLEAMS Model - A Tool for Evaluating Agrichemical Ground-Water Loading as Affected by Chemistry, Soils, Climate and Management. In: E.B. Janes and W.R. Hotchkiss (eds.), Transferring Models to Users, Denver, Colorado, November 4-8, 1990, pp. 187-197. Am. Water Resources Assoc., Bethesda, Maryland.

IGWMC Key: 6712 Model Name: CHEMFLO
Authors: Nofziger, D.L., K. Rajender, S.K. Nayudu, and P-Y. Su.
Institution of Model Development: Oklahoma State University
Dept. of Agronomy, Stillwater, Oklahoma
Code Custodian: J.R. Williams
R.S. Kerr Environm. Res. Lab., U.S. EPA, Ada, Oklahoma 74820

Abstract:

CHEMFLO is an interactive program for simulating water and chemical movement in unsaturated soils. Water movement is modeled using the Richards equation. Chemical transport is modeled by means of the convection-dispersion equation. These equations are solved numerically for one-dimensional flow and transport using finite differences. Results of the flow model can be displayed in the form of graphs of water content, matric potential, driving force, conductivity, and flux density of water versus distance or time. Graphs of concentration, and flux density of chemical as function of distance or time can also be displayed. CHEMFLO is an expansion and update of the water movement model WATERFLO by Nofziger (1985).

Model developed for: general use (e.g. in field applications), demonstration/education
Documentation includes: model theory, user's instructions, example problems
Peer (independent) review: concepts, theory (math), documentation
Availability: public domain

Remarks:

CHEMFLO is an extension and update of WATERFLO by Nofziger (1985; see IGWMC key # 6630). Soil and chemical parameters required by the model include: soil bulk density, water-soil partition coefficient, diffusion coefficient of chemical in water, dispersivity, first-order degradation rates for contaminant in the water and the solid phases, and a zero order rate constant for the liquid. Other parameters required for solving the Richards equation are the function relationships for soil-water retention and unsaturated hydraulic conductivity.

References:

Nofziger, D.L., K. Rajender, S.K. Nayudu, and P-Y Su. 1989. CHEMFLO: One-Dimensional Water and Chemical Movement in Unsaturated Soils. EPA/600/8-89/076, U.S. Environm. Protection Agency, R.S. Kerr Environm. Research Lab., Ada, Oklahoma.

IGWMC Key: 6390 Model Name: MOUSE
Authors: Pacenka, S., and T. Steenhuis
Institution of Model Development: Cornell University, Agricultural Eng. Dept., Ithaca, New York

Code Custodian: T. Steenhuis, Cornell University, Agric. Eng. Dept., Ithaca, New York

Abstract:

MOUSE (Method Of Underground Solute Evaluation) is developed for classroom and Cooperative Extension Service educational purposes. The model tracks soluble chemical movement in both the saturated and the unsaturated zone by coupling 1D vertical flow and transport in three-layer soils with 2D cross-sectional flow and transport in an anisotropic, heterogeneous aquifer. Surface runoff is calculated using the USDA Soil Conservation Service curve number equation. Active evapotranspiration occurs in the top layer of the soil. The finite difference model includes first-order degradation, dispersion, diffusion and convective mass movement. Furthermore, the model can handle linear equilibrium adsorption/desorption isotherms.

Model developed for:	general use (e.g. in field applications), demonstration/education
Documentation includes:	model theory, user's instructions, example problems, verification/validation
Verification/validation:	verification (analyt.solutions)
Availability:	public domain

References:

Pacenka, S, and T. Steenhuis. 1984. User's Guide for the MOUSE Computer Program. Agricultural Engineering Dept., Cornell University, Ithaca, New York.

IGWMC Key: 3411 Model Name: LEACHM

Authors: Wagenet, R.J., and J.L. Hutson
Institution of Model Development: Cornell University, Ithaca, New York
Code Custodian: J.L. Hutson
Dept. of Soil, Crop and Atmospheric Sciences, Cornell University, Ithaca, NY 14853

Abstract:

LEACHM (Leaching Estimation And CHemistry Model) refers to five versions of a simulation model which describes the water regime and the transport and fate of chemicals in the shallow unsaturated zone. The Richard's equation and the convective-dispersive transport equations are solved for multilayered soil profiles under transient flow conditions using finite differences. The models handle plant uptake of water and solutes, and multiple rainfall and surface evaporation cycles. The models are organized on a modular basis with separate routines for each of the simulated processes.

LEACHN describes nitrogen transport and transformation. It includes the transport of urea, ammonium and nitrate accounting for (linear) sorption, sources and sinks. The model includes diffusion in the gas phase if the chemical is volatile. Nitrogen transformations include three mineralization reactions, nitrification, and denitrification. Plant uptake of nitrogen can be simulated using Watts and Hanks approach or the Nye/Warncke approach.

LEACHP simulates movement and fate of pesticides and other miscible organic compounds accounting for linear sorption on the solid phase and diffusion in the gas phase. It can simulate the fate of many chemicals simultaneously. The various species may be grouped in degradation or transformation pathways. Pesticides can be applied in wet or dry form to the soil surface. The program allows for oxidation and hydrolysis reactions.

LEACHC describes the movement of the major inorganic cations an anions in soil. It calculates chemical equilibrium between solution, exchange and precipitated phases at user-specified intervals. The sink term in the transport equation is used to represent plant uptake. Because of competiveness of the multi-cation exchange process special subroutines are included for cation exchange, precipitation-dissolution, and atmospheric exchange.

LEACHB describes microbial population dynamics in the presence of a single growth-supporting substrate. Microbial growth and utilization are described by Monod-type equations. Equations for predator-prey systems in flowing water are included. The model has various options to introduce substrate and allows for an indigenous supply of substrate.

LEACHW describes the water regime only. A heat flow model producing soil temperature profiles is included in LEACHN and LEACHP.

Model developed for:	research (e.g. hypothesis/theory testing), general use (e.g. in field applications)
Documentation includes:	model theory, user's instructions, example problems, verification/validation
Verification/validation:	verification (analyt.solutions)
Peer (independent) review:	concepts, theory (math)
Availability:	public domain

References:

Wagenet, R.J., and J.L. Hutson. 1986. Predicting the Fate of Nonvolatile Pesticides in the Unsaturated Zone. Journ. of Environmental Quality, Vol. 15, pp. 315-322.

Hutson, J.L., and R.J. Wagenet. 1992. LEACHM Leaching Estimation And Chemistry Model; A Process-Based Model of Water and Solute Movement, Transformations, Plant Uptake and Chemical Reactions in the Unsaturated Zone, Version 3. Research Series No. 92-3, Dept. of Soil, Crop and Atmosph. Sciences, Cornell Univ., Ithaca, New York.

IGWMC Key: 4140 Model Name: MLSOIL/DFSOIL

Authors: Sjoreen, A.L., D.C. Kocher, G.G. Killough, and C.W. Miller.
Institution of Model Development: Oak Ridge National Laboratory, Oak Ridge, Tennessee
Code Custodian: A.L. Sjoreen
Oak Ridge National Laboratory, Health and Safety Research Division
Oak Ridge, Tennessee 37831

Abstract:

MLSOIL (Multi-Layer SOIL model) calculates an effective ground surface concentration to be used in computations of external doses. The program implements a five compartment linear-transfer model to calculate the concentrations of radionuclides in the soil following deposition on the ground surface from the atmosphere. The model considers leaching through the soil as well as radioactive decay and buildup. DFSOIL calculates the dose in air per unit concentration at 1m above the ground from each of the five soil layers used in MLSOIL and the dose per unit concentration from an infinite plane source. MLSOIL and DFSOIL are part of the Computerized Radiological Risk Investigation System (CRRIS).

Model developed for:	general use (e.g. in field applications)
Documentation includes:	model theory, user's instructions, example problems, program structure and development, code listing, verification/validation
Verification/validation:	verification (analyt.solutions)
Peer (independent) review:	concepts, theory (math), documentation
Availability:	public domain

References:

Sjoreen, A.L., D.C. Kocher, G.G. Killough, and C.W. Miller. 1984. MLSOIL and DFSOIL - Computer Code to Estimate Effective Ground Surface Concentrations for Dose Computations. ORNL-5974, Oak Ridge National Lab., Oak Ridge, Tennessee.

IGWMC Key: 4931 Model Name: TARGET-2DU

Authors: Moreno, J.L., M.I. Asgian, S.D. Lympany, and P-J. Pralong.
Institution of Model Development: Dames & Moore, Denver, Colorado
Code Custodian: Moreno, J.L.
Dames & Moore, 1125 17th Str., #1200, Denver, Colorado 80202

Abstract:

TARGET-2DU is one of five models of the TARGET series (Transient Analyzer of Reacting Groundwater and Effluent Transport). It simulates two-dimensional, variably saturated, density coupled, transient groundwater flow and solute transport using a hybrid finite difference method. The transport is based on the solution of the advective-dispersive transport equation for a single non-conservative contaminant with linear equilibrium adsorption (retardation). The solution method used is based on an iterative alternating direction implicit method.

Model developed for:	general use (e.g. in field applications)
Documentation includes:	model theory, user's instructions, example problems, program structure and development, verification/validation
Verification/validation:	verification (analyt.solutions)
Availability:	proprietary, license

References:

Dames & Moore. 1985. Physical and Mathematical Background of Two-Dimensional and Three-Dimensional Variably Saturated, Density Coupled Models. Denver, Colorado.

Dames & Moore. 1985. User's Guide to TARGET_2DU, Version 4.0. Denver, Colorado.

IGWMC Key: 4934 Model Name: TARGET-3DU

Authors: Moreno, J.L., M.I. Asgian, S.D. Lympany, and P-J. Pralong

Institution of Model Development: Dames & Moore, Denver, Colorado

Code Custodian: J.L. Moreno
Dames & Moore, 1125 17th. Str., #1200, Denver, Colorado 80202

Abstract:

TARGET-3DU is one of five models of the TARGET series (Transient Analyzer of Reacting Groundwater and Effluent Transport). It simulates three-dimensional, variably-saturated, density-coupled, transient groundwater flow and solute transport using a hybrid finite difference method. The transport is based on the solution of the advective-dispersive transport equation for a single non-conservative contaminant with linear equilibrium adsorption (retardation). The solution method used is based on an iterative alternating direction implicit method.

Model developed for:	general use (e.g. in field applications)
Documentation includes:	model theory, user's instructions, example problems, program structure and development, verification/validation
Verification/validation:	verification (analyt.solutions)
Availability:	proprietary, license

References:

Dames & Moore. 1985. Physical and Mathematical Background of Two-Dimensional and Three-Dimensional Variably Saturated, Density Coupled Models. Denver, Colorado.

Dames & Moore. 1985. User's Guide to TARGET-3DU, Version 4.0. Denver, Colorado.

IGWMC Key: 4693 Model Name: VADOFT
Authors: Huyakorn, P.S., T.D. Wadsworth, H.O. White Jr., and J.E. Buckley
Institution of Model Development: Hydrogeologic, Inc., Herndon, Virginia
Code Custodian: Jan Kool
Hydrogeologic, Inc., 1165 Herndon Parkway, #900, Herndon, VA 22070

Abstract:

VADOFT is a one-dimensional finite element code that solves the Richard's equation for flows in the unsaturated zone. The user may make use of constitutive relationships between pressure, water content, and hydraulic conductivity to solve the flow equations. VADOFT also simulates the fate and transport of two parent and two daughter products.

Model developed for: research (e.g. hypothesis/theory testing), general use (e.g. in field applications)
Availability: public domain

Remarks:

PRZM, VADOFT and SAFTMOD are part of RUSTIC. RUSTIC (IGWMC Key # 4721) links these models in order to predict the fate and transport of chemicals to drinking water wells. The codes are linked together with the aid of a flexible execution supervisor (software user interface) that allows the user to build models that fit site-specific situations.

References:

Huyakorn, P.S., T.D. Wadsworth, H.O. White, Jr., and J.E. Buckley. 1987. 'VADOFT' Version 3.2, Project Report for USEPA, Environm. Research Lab., Athens, Georgia. Hydrogeologic, Inc., Herndon, Virg.

See also references of RUSTIC (IGWMC # 4721).

IGWMC Key: 5186 Model Name: NITRO
Authors: Kaluarachchi, J.J., and J.C. Parker
Institution of Model Development: Environmental Systems & Technologies, Inc., Blacksburg, Virginia

Code Custodian: J.C. Parker
Environmental Systems & Technologies, Inc.
P.O. Box 10457, Blacksburg, VA 24062-0457

Abstract:

NITRO is a 2-dimensional vertical section or radially symmetric finite element program for simulation of steady-state and transient uncoupled flow and transport in the unsaturated zone. The nonlinearity is handled by Picard iteration. Soil hydraulic properties are described by the Brooks-Corey or van Genuchten model with hysteresis. The model handles transport of up to two species with linear or Freundlich equilibrium adsorption and zero and first order transformations. It facilitates atmospheric and seepage boundaries as well as first-type and second-type (flux) boundary conditions.

Model developed for: research (e.g. hypothesis/theory testing), general use (e.g. in field applications)
Documentation includes: user's instructions, example problems
Availability: proprietary, license

IGWMC Key: 5220 Model Name: VSAFT2 (Variably SAturated Flow and Transport in 2 dimensions)
Authors: Yeh, T-C.J.
Institution of Model Development: The University of Arizona, Dept. of Hydrology and Water Resources Tuscon, Arizona
Code Custodian: T-C.J. Yeh
Dept. of Hydrology and Water Resources
University of Arizona, College of Engineering and Mines
Building 11, Tuscon, AZ 85721

Abstract:

VSAFT2 is a program for simulating two-dimensional steady or transient, variably saturated flow and convective-dispersive transport of a conservative solute, using a finite element method with the Newton-Raphson or Picard iteration scheme. For the linear equation solution a preconditioned conjugate gradient method is used. Solute transport is handled by an upstream weighing scheme. The model uses rectangular and/or triangular finite elements and a banded matrix solver. The two-dimensional flow can be either in a horizontal or in a vertical plane. Furthermore, the model can handle radial symmetric simulations. The code contains a restart feature for changing boundary conditions.

Model developed for: research (e.g. hypothesis/theory testing)
Documentation includes: model theory, user's instructions, example problems, program structure and development, code listing, verification/validation
Verification/validation: verification (analyt.solutions), code intercomparison
Availability: public domain

Remarks:

Evapotranspiration is simulated in VSAFT2 by a user specified root zone consisting of one or more plant species. User supplied information on the root zone includes wilting pressure, maximum transpiration rate, root effectiveness function, and root zone geometric data. Evaporation \ Infiltration is simulated through user defined maximum evaporation or infiltration rates, minimum soil surface pressure head, and soil surface geometric data. Analytical functions must be used for relative hydraulic conductivity relationships and moisture characteristic curve functions. The user is given the choice of the van Genuchten model, exponential model, Gardener-Russo model, or a user specified function for which a subroutine must be written.

Documentation includes test problems where results from VSAFT2 are compared to UNSAT2, FEMWATER/FEMWASTE, VAM2D, and VADOFT.

References:

Yeh, T-C.J., and R. Srivastava. 1990. VSAFT2: Variably Saturated Flow and Transport in 2-Dimensions; a Finite Element Simulation. Technical Report No. HWR 90-010, Dept. of Hydrology & Water Resources, The University of Arizona, Tuscon, Arizona.

IGWMC Key: 5221 Model Name: VSAFT3 (Variably SAturated Flow and Transport in 3 dimensions)
Authors: Srivastava, R. and T-C.J. Yeh
Institution of Model Development: The University of Arizona, Dept. of Hydrology and Water Resources Tuscon, Arizona
Code Custodian: T.C.J. Yeh
Dept. of Hydrology and Water Resources, Univ. of Arizona
Building 11, Tuscon, AZ 85721

Abstract:

VSAFT3 is a three-dimensional finite element model for simulation of transient flow and convective-dispersive transport in variably saturated porous media. The resulting flow matrix equations are solved using a Picard iteration scheme and a continuous velocity field is obtained by separate application of the Galerkin technique to the flux equation. A two-site adsorption-desorption model with first-order loss term is used for the reactive solute. The advective part of the transport equation is solved with one-step backwards particle tracking (MMOC), while the dispersive part is solved using the regular Galerkin finite element technique. The resulting matrix equations are solved with a PGJ method. The code contains a restart feature for changing boundary conditions.

Model developed for:	research (e.g. hypothesis/theory testing)
Documentation includes:	model theory, user's instructions, example problems, program structure and development, code listing, verification/validation
Verification/validation:	verification (analyt.solutions), code intercomparison
Availability:	public domain

References:

Srivastava, R., and T-C.J. Yeh. 1992. A Three-Dimensional Numerical Model for Water Flow and Transport of Chemically Reactive Solute Through Porous Media under Variably Saturated Conditions. Submitted to Adv. in Water Resources.

IGWMC Key: 4721 Model Name: RUSTIC

Authors: Dean, J.D., P.S. Huyakorn, A.S. Donigan, Jr., K.A. Voos, R.W. Schanz, Y.J. Meeks, and R.F. Carsel

Institution of Model Development: Woodward-Clyde Consultants, Oakland, California

Code Custodian: R.F. Carsel
U.S. Environmental Protection Agency
Environmental Research Laboratory, Athens, GA 30613

Abstract:

RUSTIC is a coupled root zone (PRZM), unsaturated zone (VADOFT), and saturated zone (SAFTMOD) modeling package. RUSTIC links these models in order to predict the fate and transport of chemicals to drinking water wells. The codes are linked together with the aid of a flexible execution supervisor (software interface) that allows the user to build models that fit site-specific situations. For exposure assessments, the code is equipped with a Monte Carlo pre- and post-processor.

Model developed for:	research (e.g. hypothesis/theory testing), general use (e.g. in field applications)
Availability:	public domain

Remarks:

PRZM (MARS Key # 4720) is a one-dimensional finite difference model which accounts for pesticide fate and transport in the crop root zone. The version included in RUSTIC incorporates several features added to the original code, such as soil temperature effects, volatilization and vapor phase transport in soils, irrigation simulation and a method of characteristics algorithm to eliminate numerical dispersion. This PRZM version is capable of simulating fate and transport of the parent and up to two daughter species.

VADOFT (MARS Key # 4693) is a one-dimensional finite element code that solves the Richard's equation for flows in the unsaturated zone. The user may make use of constitutive relationships between pressure, water content, and hydraulic conductivity to solve the flow equations. VADOFT also simulates the fate and transport of two parent and two daughter products.

SAFTMOD (MARS Key # 4694) is a two-dimensional finite element model that simulates saturated solute flow and transport in either X-Y or X-Z configuration.

References:

Dean, J.D., P.S. Huyakorn, A.S. Donigan, Jr., K.A. Voos, R.W. Schanz, Y.J. Meeks, and R.F. Carsel. 1989. Risk of Unsaturated/Saturated Transport and Transformation of Chemical Concentrations (RUSTIC); Volume 1: Theory and Code Verification. EPA/600/3-89/048a, U.S. EPA, ORD/ERL, Athens, Georgia.

Dean, J.D., P.S. Huyakorn, A.S. Donigan, Jr., K.A. Voos, R.W. Schanz, Y.J. Meeks, and R.F. Carsel. 1989. Risk of Unsaturated/Saturated Transport and Transformation of Chemical Concentrations (RUSTIC); Volume 2: User's Guide. EPA/600/3-89/048b, U.S. EPA, ORD/ERL, Athens, Georgia.

IGWMC Key: 5630 Model Name: MULTIMED

Authors: Salhotra, A.M., P. Mineart, S. Sharp-Hansen, and T. Allison

Institution of Model Development: U.S. EPA, Environmental Res. Lab., Athens, Georgia

Code Custodian: Center for Exposure Assessment Modeling
U.S. Environmental Protection Agency
Environmental Research Lab., College Station Road,
Athens, GA 30613

Abstract:

MULTIMED is a multimedia transport model that simulates the movement of contaminants leaching from a waste disposal facility. The model includes two options or simulating leachate flux. Either the infiltration rate to the unsaturated or saturated zone can be specified directly or a landfill module can be used to estimate the infiltration rate. The landfill module is one-dimensional and steady-state, and simulates the effect of precipitation, runoff, infiltration, evapotranspiration, barrier layers (which can include flexible membrane liners), and lateral drainage. A steady-state, one-dimensional, semi-analytical module simulates flow in the unsaturated zone. The output from this module, water saturation as function of depth, is used as input to the unsaturated transport module. The unsaturated transport module simulates transient, one-dimensional (vertical) transport and includes the effects of longitudinal dispersion, linear adsorption, and first-order decay. Output from this module -i.e. steady-state or time-varying concentrations at the water table- is used to couple the unsaturated zone transport module with a steady-state or transient, semi-analytical saturated zone transport module. The saturated zone transport model of MULTIMED includes one-dimensional uniform flow, three-dimensional dispersion, linear adsorption (retardation), first-order decay, and dilution due to direct infiltration into the ground water plume. Contamination of a surface stream due to the complete interception of a steady-state saturated zone plume is simulated by the surface water module. Finally, the air emissions and the atmosphere dispersion modules simulate the movement of chemicals into the atmosphere. The module includes option for Monte Carlo simulations.

Model developed for: research (e.g. hypothesis/theory testing), general use (e.g. in field applications)

Availability: public domain

References:

Salhotra, A.M., P. Mineart, S. Sharp-Hansen, and T. Allison. 1990. Multimedia Exposure Assessment Model (MULTIMED) for Evaluating the Land Disposal of Wastes -- Model Theory. Report Contract # 68-03-3513 and 68-03-6304, U.S. EPA, Env. Res. Lab., Athens, Georgia.

Sharp-Hansen, S., C. Traverse, P. Hummel, and T. Allison. 1990. A Subtitle D Landfill Application Manual for the Multimedia Exposure Assessment Model (MULTIMED). Report Contract # 68-03-3513, U.S. EPA, Env. Res. Lab., Athens, Georgia.

IGWMC Key: 5310 Model Name: PRZMAL

Authors: Wagner, J., and C. Ruiz-Calzada

Institution of Model Development: Oklahoma State University
School of Chemical Engineering, Stillwater, Oklahoma

Code Custodian: J. Wagner
Oklahoma State University, School of Chemical Engineering, Stillwater, OK 74074

Abstract:

PRZMAL is an aquifer linkage model for US EPA's Pesticide Root Zone Model (PRZM). It connects PRZM with the analytical three-dimensional transport model PLUME 3D developed at Oklahoma State University. This linkage allows the user to predict contaminant movement from the point of application, in a continuous manner, into and within the aquifer.

Model developed for: general use (e.g. in field applications)
Documentation includes: model theory, user's instructions
Availability: public domain

Remarks:

PRZM (MARS Key # 4720) is a one-dimensional finite difference model which accounts for pesticide fate and transport in the crop root zone. It includes soil temperature effects, volatilization and vapor phase transport in soils, irrigation simulation and a method of characteristics algorithm to eliminate numerical dispersion. PRZM is capable of simulating fate and transport of the parent and up to two daughter species.

Wagner and Ruiz designed an aquifer linkage model PRZMAL to connect PRZM with the analytical three-dimensional model PLUME 3D.

References:

Wagner, J., and C. Ruiz-Calzada. 1986. User's Manual for PRZM-Aquifer (PRZMAL). Oklahoma State University, School of Chemical Engineering, Stillwater, Oklahoma.

IGWMC Key: 5681 Model Name: VIP (Vadose zone Interactive Processes model)

Authors: Stevens, D.K., W.J. Grenney, and Z. Yan

Institution of Model Development: Civil and Environm. Eng., Utah State Univ., Logan, Utah

Code Custodian: D.K. Stevens
Civil and Environm. Eng. Dept., Utah State Univ., UMC 4110, Logan, Utah 84321

Abstract:

VIP is an one-dimensional finite-difference solute transport and fate model for simulating the behavior of organic (oily) compounds in the vadose zone as part of a land treatment system. The model uses advection and dispersion in the water and air phases as the dominant transport mechanism for contaminant and oxygen. Monthly values for recharge rate and soil moisture conditions are used to calculate an effective water velocity. The model includes first-order degradation of a contaminant in water, air and soil, and of oxygen. It uses an implicit technique to calculate the degradation of the contaminant in the oil phase as well as the oil phase itself, and related oxygen changes. (see also remarks).

Model developed for:	research (e.g. hypothesis/theory testing), general use (e.g. in field applications)
Documentation includes:	model theory, user's instructions, example problems, program structure and development, and verification/validation
Verification/validation:	laboratory data sets, field datasets (validation)
Peer (independent) review:	concepts, theory
Availability:	public domain

Remarks:

VIP uses partition coefficients and rate constants to calculate contaminant concentration in each medium. The model has various output options including echo of input data, (graphic) profile of initial condition (constituent concentration in water, oil, air, and soil phases), and the initial fractions as well as initial oxygen concentration. Other output options include (graphic) depth-concentration profiles and data versus time tables. Input preparation facilitates exchange of Lotus 123 and wordprocessed ASCII files.

This software is available from: Center for Subsurface Modeling Support (CSMOS), R.S. Kerr Environmental Research Laboratory, U.S. Environmental Protection Agency, P.O. Box 1198, Ada, OK 74820, Phone: 405/332-8800.

References:

Stevens, D.K. W.J. Grenney, and Z. Yan. 1991. A Model for the Evaluation of Hazardous Substances in the Soil. Version 3.0. Civil and Environm. Eng. Dept., Utah State Univ., Logan, Utah.

Grenney, W.J., G.L. Caupp, R.C. Sims, and T.E. Short. 1987. A Mathematical Model for the fate of Hazardous Substances in Soil: Model Description and Experimental Results. Haz. Waste & Haz. Mat., Vol. $(3), pp. 223-239

IGWMC Key: 5850 Model Name: RZWQM (Root Zone Water Quality Model)

Authors: DeCoursey, D.G., K.W. Rojas, and L.R. Ahuja

Institution of Model Development: USDA-ARS, Fort Collins, Colorado

Code Custodian: Lajpat R. Ahuja
Agricultural Research Service, U.S. Dept. of Agric., Hydro-Ecosystems Research Group, P.O. Box E, Fort Collins, CO 80522

Abstract:

RZWQM is a physically based model simulating the movement of water, nutrients, and pesticides over and through the root zone at a representative point in a field. The physical processes included are soil matrix infiltration, macropore flow, surface runoff, heat flow, potential evaporation, and transpiration, soil-water

redistribution and chemical transport. Root water uptake, actual evaporation and transpiration, are calculated in the crop growth section in conjunction with water redistribution and plant growth. Soil chemical processes include bicarbonate buffering, dissolution and precipitation of calcium carbonate, gypsum, and aluminum hydroxide, ion exchange involving bases and aluminum, and solution chemistry of aluminum hydroxide. (see also remarks).

Model developed for:	general use (e.g. in field applications), demonstration/education
Documentation includes:	user's instructions
Verification/validation:	under development (as of 7/'92)
Peer (independent) review:	under development
Availability:	public domain; test version only

Remarks:

RZWQM also includes various nutrient processes such as decomposition of organic matter, mineralization, immobilization and demineralization of appropriate nitrogen and phosphorus species, and adsorption/desorption of both species. Pesticide processes the model can handle include computation of the amount of pesticides reaching the soil surface, and the amounts absorbed and moving through each soil layer. Dissipation via volatilization, photolysis, hydrolysis, biodegradation, oxidation, and complexation are simulated. These processes may be lumped in a single process.

Other pesticide related processes simulated in RZWQM are dissipation by formulation of metabolites (tracked throughout their life time). Either equilibrium isotherms or kinetic adsorption/desorption processes may be simulated. The model allows to include certain management practices such as effects of tillage practices on chemical distribution, soil density, and macro- and microporosity; fertilizer and pesticide applications; planting densities; and irrigation and drainage practices.

References:

Hebson, C.S., and D.G. DeCoursey. 1987. A Model for Assessing Management Impact on Root-Zone Water Quality. In: Proceed. Am. Chem. Soc. 193rd. Nat. Meeting, Agro Chemicals Div., Denver, Colorado, April 5-10, 1987.

Hebson, C.S., and D.G. DeCoursey. 1987. A Model for Ranking Land-Use Management Strategies to Minimize Unsaturated Zone Contamination. In: Proceed. ASCE Eng. Hydrology Symposium, Williamsburg, Virginia, August 3-5, 1987.

IGWMC Key : 6221 Model Name: SWMS-2D

Authors: Simunek, J., T. Vogel and M.Th. van Genuchten

Institution of Model Development: U.S. Salinity Laboratory, Agricultural Research Service
Dept. of Agriculture, Riverside, Calif.

Code Custodian: M.Th. van Genuchten
Institution: U.S. Salinity Laboratory, Agricultural Research Service
U.S. Dept. of Agriculture, 4500 Glenwood Drive, Riverside, CA 92501

Abstract:

The program 'SWMS_2D' is a numerical model for simulating water and solute movement in two-dimensional variably saturated media. The program numerically solves the Richards' equation for saturated-unsaturated water flow and the advection-dispersion equation for solute transport. The flow equation incorporates a sink term to account for water uptake by plant roots. The transport equation includes provisions for linear equilibrium adsorption, zero-order production and first-order degradation. The program may be used to analyze water and solute movement in unsaturated, partially saturated, or fully saturated porous media.

SWMS_2D can handle flow regions delineated by irregular boundaries. The flow region itself may be composed of nonuniform soils having an arbitrary degree of local anisotropy. Flow and transport can occur in the vertical plane, the horizontal plane, or in a three-dimensional region exhibiting radial symmetry about the vertical axis. The water flow part of the model can deal with (constant or varying) prescribed head and flux boundaries, as well as boundaries controlled by atmospheric conditions. Soil surface boundary conditions may change from prescribed flux to prescribed head type conditions (and vice-versa). The code can also handle a seepage face boundary through which water leaves the saturated part of the flow domain.

For solute transport the code supports both (constant and varying) prescribed concentration (Dirichlet or first-type) and concentration flux (Cauchy or third-type) boundaries. The dispersion tensor includes a term reflecting the effects of molecular diffusion and tortuosity.

The unsaturated soil hydraulic properties are described by a set of closed-form equations resembling the 1980 van Genuchten equations. Modifications were made to improve the description of hydraulic properties near saturation. SWMS_2D implements a scaling procedure to approximate the hydraulic variability in a given area by means of a set of linear scaling transformations which relate the individual soil hydraulic characteristics to reference characteristics.

The governing equations are solved using a Galerkin type linear finite element method applied to a network of triangular elements. Integration in time is achieved using an implicit (backwards) finite difference scheme for both saturated and unsaturated conditions. The resulting equations are solved in an iterative fashion, by linearization and subsequent Gaussian elimination. Additional measures are taken to improve solution efficiency in transient problems, including automatic time step adjustment and checking if the Courant and Peclet numbers do not exceed a preset level. The water content term is evaluated using the mass-conservative method proposed by Celia et al. (1990). To minimize numerical oscillations upstream weighing is included as an option for solving the transport equation.

Model developed for:	research (e.g. hypothesis/theory testing), general use (e.g. in field applications), demonstration/education
Documentation includes:	model theory, user's instructions, example problems, program structure and development, code listing, and verification/validation
Verification/validation:	verification (analyt.solutions), laboratory data sets, code intercompariosn
Peer (independent) review:	concepts, theory (math), documentation

References

Simunek, J., T. Vogel and M.Th. van Genuchten. 1992. The SWMS_2D Code for Simulating Water Flow and Solute Transport in Two-Dimensional Variably Saturated Media; Version 1.1. Research Report 126, U.S. Salinity Laboratory, USDA/ARS, Riverside, California.

IGWMC Key : 6229 Model Name: HYDRUS/WORM

Authors: Kool, J.B., M.Th. van Genuchten
Institution of Model Development: U.S. Salinity Laboratory, Agricultural Research Service
Dept. of Agriculture, Riverside, Calif.
Code Custodian: M.Th. van Genuchten
Institution: U.S. Salinity Laboratory, Agricultural Research Service
U.S. Dept. of Agriculture, 4500 Glenwood Drive, Riverside, CA 92501

Abstract:

HYDRUS is a Galerkin linear finite element program for simulation of transient one-dimensional flow and solute transport in variably saturated porous media. The solution of the flow problem considers the effects

of root uptake and hysteresis in the soil hydraulic properties. The solute transport equation incorporates the processes of ionic or molecular diffusion, hydrodynamic dispersion, linear or nonlinear equilibrium adsorption, and first-order decay. Boundary conditions for the flow and transport may be constant or time-varying. For flow boundary conditions, HYDRUS can solve the steady-state flow equation in a single step without the need of performing time-marching.

The solution of the flow equation in HYDRUS requires specification of the initial condition in terms of pressure head or water content. Either first- or second-type boundary conditions can be imposed at the soil surface. Alternatively, the upper boundary condition may be specified in terms of total amount of surface applied water, combining both types of boundary conditions. The auxiliary condition at the lower boundary is given in terms of imposed pressure head, zero head gradient, or imposed net drainage flux. Type of boundary condition might change in time.

Soil hydraulic properties in HYDRUS can be described by the parametric functions of Van Genuchten (1978). Uptake of water by plant roots includes evapotranspiration, a normalized root uptake distribution function, and a pressure-salinity stress response function. HYDRUS uses the fully-implicit scheme to solve the set of matrix equations for flow and transport. Nonlinearities in the flow equations are treated using Picard iteration with under-relaxation. For solute transport, corrections are applied to the dispersion coefficient to reduce numerical problems.

The HYDRUS program is a modification of the WORM program developed at the U.S. Salinity Laboratory.

Model developed for:	research (e.g. hypothesis/theory testing), general use (e.g. in field applications), demonstration/education
Documentation includes:	model theory, user's instructions, example problems, program structure and development, code listing, and verification/validation
Verification/validation:	verification (analyt.solutions), laboratory data sets
Peer (independent) review:	concepts, theory (math), documentation

References

Kool, J.B., and M.Th. van Genuchten. 1991. HYDRUS. One-Dimensional Variably Saturated Flow and Transport Model Including Hysteresis and Root Water Uptake. U.S. Salinity Lab., U.S. Dept. of Agric., Agric. Res. Service, Riverside, Calif.

Appendix 4: Solute Transport in the Unsaturated Zone (requiring given head distribution)

IGWMC Key: 4350 Model Name: FEMTRAN
Author: Martinez, M.J.
Institution of Model Development: Sandia National Laboratories
Albuquerque, New Mexico
Code Custodian: Mario Martinez
Sandia National Laboratories, Fluid Mechanics and Heat Transfer Div.
Albuquerque, NM 87185

Abstract:

FEMTRAN is a two-dimensional finite element model to simulate cross-sectional advective radionuclide transport in saturated/unsaturated porous media. The model considers chain-decay of the radionuclides. It requires user prescribed heads.

Model developed for:	research (e.g. hypothesis/theory testing), general use (e.g. in field applications)
Documentation includes:	model theory, user's instructions, example problems, program structure and development, verification/validation
Verification/validation:	verification (analyt.solutions)
Peer (independent) review:	concepts, theory (math)
Availability:	public domain

Remarks:

This model is based on a code developed by Duguid and Reeves (1976) and later updated by Yeh and Ward at Oak Ridge National Laboratory (FEMWASTE; IGWMC Key # 3371).

References:

Martinez, M.J. 1985. FEMTRAN - A Finite Element Computer Program for Simulating Radionuclide Transport through Porous Media. SAND84-0747, Sandia National Lab., Albuquerque, New Mexico.

IGWMC Key: 3371 Model Name: FEMWASTE/FECWASTE
Authors: Yeh, G.T., and D.S. Ward
Institution of Model Development: Oak Ridge National Laboratory
Oak Ridge, Tennessee
Code Custodian: G.T. Yeh
Penn State University, Dept. of Civil Eng.
225 Sackett Bldg, University Park, PA 16802

Abstract:

FEMWASTE/FECWASTE are two-dimensional finite element models for transient simulation of areal or cross-sectional transport of dissolved non-conservative constituents for a given velocity field in an anisotropic, heterogeneous saturated or unsaturated porous medium. The velocity field is generated by the accompanying FEMWATER/FECWATER two-dimensional flow models.

Model developed for:	research (e.g. hypothesis/theory testing), general use (e.g. in field applications)
Documentation includes:	model theory, user's instructions, example problems, verification/validation
Verification/validation:	verification (analyt.solutions)

Peer (independent) review: concepts, theory (math)
Availability: public domain

Remarks:

FEMWASTE is a modified and updated version of a model published by Duguid and Reeves in 1976. FECWASTE is a slightly modified and updated version of FEMWASTE. FEMWASTE and FECWASTE use the velocity field generated by the models FEMWATER and FECWATER, respectively (IGWMC key # 3370).

References:

Yeh, G.T. and D.S. Ward. 1981. FEMWASTE: A Finite-Element Model of a Waste Transport through Porous Media. ORNL-5601. Oak Ridge Nat. Lab., Oak Ridge, Tenn.

Yeh, G.T. and R.H. Strand. 1982. FECWASTE: Users' Manual of a Finite-Element Computer Code for Simulating Waste Transport through Saturated-Unsaturated Porous Media. ORNL/TM-7316. Oak Ridge Nat. Lab., Oak Ridge, Tenn.

Duguid J. and M. Reeves. 1976. Material Transport through Saturated-Unsaturated Porous Media: A Galerkin Finite Element Model. ORNL-4928. Oak Ridge Nat. Lab., Oak Ridge, Tenn.

Yeh, G.T. 1982. Training Course No.2: The Implementation of FEMWASTE (ORNL-5601) Computer Program. Oak Ridge Nat Lab., Oak Ridge, Tenn.

Yeh, G.T. 1982. Training Course No.2: The Implementation of FEMWASTE (ORNL-5601) Computer Program. NUREG/CR-2706, U.S. Nuclear Regulatory Commission, Washington, D.C.

IGWMC Key: 6130 Model Name: PESTAN

Authors: Enfield, C.G., R.F. Carsel, S.Z. Cohen, and T. Phan
Institution of Model Development: R.S. Kerr Environm. Res. Lab., U.S. EPA
Ada, Oklahoma.
Code Custodian: Center for Subsurface Modeling Support (CSMOS)
R.S. Kerr Environm. Res. Lab., U.S. EPA
P.O. Box 1198, Ada, Oklahoma 74820

Abstract:

PESTAN (PESticide Analytical Model) is an interactive analytical model, used for estimating organic chemical movement in the unsaturated zone. The model is based on an analytical solution of the convective dispersive solute transport equation for single layer homogeneous soils. It calculates vertical convective movement of chemicals with linear equilibrium sorption and first-order (bio-) chemical decay. Hydrologic loading is based on annual water balance. The primary application has been for pesticide screening.

Model developed for: research (e.g. hypothesis/theory testing), general use (e.g. in field applications)
Documentation includes: model theory, user's instructions, example problems, verification/validation
Verification/validation: verification (analyt.solutions)
Peer (independent) review: concepts, theory (math)
Availability: public domain

Remarks:

This model is available from the International Ground Water Modeling Center, Colorado School of Mines, Golden, CO 80401, USA.

References:

Enfield, D.G., R.F. Carsel, S.Z. Cohen, T. Phan, and D.M. Walters. 1982. Approximating Pollutant Transport to Ground Water. Ground Water, Vol. 20(6), pp. 711-722.

Donigian, Jr., A.S., and P.S.C. Rao. 1986. Overview of Terrestrial Processes and Modeling. In: S.C. Hern and S.M. Melancon (eds.), Vadose Zone Modeling of Organic Polllutants. Lewis Publishers, Chelsea, Michigan.

IGWMC Key: 6225 Model Name: CHAIN
Authors: van Genuchten, M. A.
Institution of Model Development: USDA Salinity Lab., Riverside, Calif.

Code Custodian: M.Th. van Genuchten
USDA Salinity Laboratory, 4500 Glenwood Drive, Riverside, CA 92501

Abstract:

The CHAIN model simulates multi-ion transport across the unsaturated zone using an analytical procedure. The model includes longitudinal dispersion and first-order decay. It calculates the time history of chemical concentration exiting the unsaturated zone.

Model developed for:	research (e.g. hypothesis/theory testing)
Documentation includes:	model theory, user's instructions, example problems, program structure and development, verification/validation
Verification/validation:	laboratory data sets
Peer (independent) review:	concepts, theory (math)
Availability:	public domain

IGWMC Key: 5620 Model Name: SUMMERS
Authors: Summers, K., S. Gherini, and C. Chen
Institution of Model Development: Tetra Tech, Inc., Lafayette, Calif.

Code Custodian: U.S. Environmental Protection Agency
Environmental Research Laboratory, Athens, GA 30613

Abstract:

The SUMMERS model refers to a combination of an analytical solution for one-dimensional, non-dispersive transport in soil due the continuous release at the surface, and a mass-balance evaluation of the subsequent mixing in an underlying aquifer. This model can be used to estimate the contaminant concentrations in the soil which will produce ground-water contaminant concentrations above acceptable levels. The resultant soil concentrations can then be used as guidelines in estimating boundaries or extent of soil contamination and specifying soil cleanup goals for remediation. The model utilizes steady-state water movement and equilibrium partitioning of the contaminant in the unsaturated zone. For assessment of the concentration in the aquifer, the model assumes a constant flux from the surface source to the aquifer and instantaneous, complete mixing in the aquifer. The model does not account for volatilization, and should not be used for volatile compounds.

Model developed for: general use (e.g. in field applications)
Availability: can be coded by user

References:

Summers, K., S. Gherini, and C. Chen. 1980. Methodology to Evaluate the Potential for Ground Water Contamination from Geothermal Fluid Releases; pp. 67-73. EPA-600/7-80-117, U.S. EPA, ORD/IERL, Cincinnati, Ohio.

IGWMC Key: 5661 Model Name: FLAME

Authors: Baca, R.G., and S.O. Magnuson
Institution of Model Development: Idaho Nat. Eng. Lab., EG&G, Idaho Falls, Idaho

Code Custodian: Baca, R.G.
Idaho Nat. Eng. Lab., EG&G Idaho, Inc., P.O. Box 1625, Idaho Falls, Idaho 83415

Abstract:

FLAME is a finite element code designed to simulate two-dimensional, cross-sectional subsurface transport of low-concentration contaminants in either time-dependent or steady-state, known flow field in a highly heterogeneous variably-saturated porous media with complex stratigraphy. The code can be applied to two-dimensional transport in an arid vadose zone or in an unconfined aquifer. FLAME handles advective-dispersive transport, equilibrium sorption using a linear isotherm, first-order decay, and a complex source/sink term. It accommodates advection-dominated mass transport. In addition, the code has the capability to describe transport processes in a porous media with discrete fractures. It describes the mass transfer between the porous media and discrete fractures.

Model developed for: general use (e.g. in field applications)
Documentation includes: model theory, user's instructions, example problems, verification/validation
Verification/validation: verification (analyt.solutions), code intercomparison
Peer (independent) review: concepts, theory (math)

Remarks:

FLAME can handle both Dirichlet and Neumann transport boundary conditions. The code can model transport of contaminants in a single phase, being either liquid, gaseous (e.g. organic vapors), or colloidal. The modified equation approach of Fletcher with a build-in dissipation mechanism is used to dampen oscillations in a convection dominated transport system. The resulting finite element matrix equations are solved by a Gaussian elimination procedure without pivoting. Two solvers are used: 1) standard band solver utilizing a skyline storage scheme, and 2) frontal method.

References:

Baca. R.G., and S.O. Magnuson. 1988. FLAME - A Finite Element Computer Code for Contaminant Transport in Variably-Saturated Media. EGG-GEO-10329, Idaho Nat. Eng. Lab., EG&G, Idaho Falls, Idaho.

IGWMC Key: 5690 Model Name: VLEACH (Vadose Zone LEACHing Model)
Author: J. Turin
Institution of Model Development: CH2M-Hill, Reading, Calif.

Code Custodian: see remarks

Abstract:

VLEACH is a relatively simple one-dimensional finite difference model designed to simulate leaching of a volatile, adsorbed contaminant through the vadose zone. It can be used to simulate the transport of any non-reactive chemical that displays linear partitioning behavior. In particular, VLEACH simulates downward liquid-phase advection, solid-phase sorption, gas diffusion in the vapor phase, and three-phase equilibrium. The contaminant mass within each model cell is partitioned among liquid (dissolved in water), vapor, and solid phases. The model assumes a homogeneous porous medium with steady flow and no dispersion. There is no in-situ degradation or production, and free product is not present.

Model developed for:	general use (e.g. in field applications)
Documentation includes:	model theory, user's instructions, example problems, and program structure and development.
Availability:	public domain

Remarks:

Input data for VLEACH consists of: organic carbon coefficient (Koc), Henry's Law constant (Kh), the aqueous solubility and the free air diffusion coefficient. The input soil properties are dry bulk density, total porosity, volumetric water content and organic carbon fraction, and site-specific input parameters such as recharge rate and depth to groundwater.

This software is available from: Center for Subsurface Modeling Support (CSMOS), R.S. Kerr Environmental Research Laboratory, U.S. Environmental Protection Agency, P.O. Box 1198, Ada, OK 74820, Phone: 405/332-8800.

References:

Turin, J. August 1990. VLEACH: A One-Dimensional Finite Difference Vadose Zone Leach Model. Report prepared for U.S. EPA, Region 9., CH2M Hill, Reading, Calif.

Appendix 5: Flow and Heat Transport in the Unsaturated Zone

IGWMC Key: 2582 Model Name: TOUGH (Transport of Unsaturated Groundwater and Heat)

Authors: Pruess, K., Y.W. Tsang, and J.S.Y. Wang
Institution of Model Development: Lawrence Berkeley Laboratory
Berkeley, California
Code Custodian: Pruess, K.
Lawrence Berkeley Laboratory, Earth Science Division
Mailstop 50E LBL, University of California
Berkeley, CA 94720

Abstract:

TOUGH is a multi-dimensional integrated finite difference model for transient simulation of the coupled transport of water, air, vapor and heat transport in fractured unsaturated porous media. The model includes convection, condensation, capillary forces, evapotranspiration, heat conduction and diffusion, change of phase, adsorption, fluid compression, dissolution of air in liquid, and buoyancy. The gas and liquid phase flow of air and water, and heat transport are solved in a fully coupled manner.

Model developed for:	research (e.g. hypothesis/theory testing)
Documentation includes:	model theory, user's instructions, example problems, program structure and development, code listing, verification/validation
Verification/validation:	verification (analyt.solutions), laboratory data sets, code intercomparison
Peer (independent) review:	concepts, theory (math), documentation
Availability:	public domain

Remarks:

The TOUGH code is available with full documentation from:
National Energy Software Center (NESC)
Argonne National Lab.
9700 South Cass Ave., Argonne, IL 60439

To evaluate how hysteretic capillary pressure-liquid saturation relation may effect the flow and liquid saturation distribution in a fractured rock system, Niemi and Bodvarsson (1988; see references) included capillary hysteresis in the numerical flow simulator TOUGH. Material properties used for these evaluations represent the densely welded tuff of the Yucca Mountain site in Nevada.

A fracture network generator based on the MINC concept is available for TOUGH (see Pruess, 1983).

TOUGH was tested by Sandia National Laboratories and results were compared to analytical solutions, laboratory data sets, and the programs NORIA and PETROS. TOUGH was capable of solving most of the problems and out-performed the other codes. However, it had the most difficulty with numerical dispersion. TOUGH'S greatest weakness is the way it handles boundary conditions especially when boundary conditions are mixed in the form of prescribed mass flux and constant temperature (or similar conditions).

Relative permeability must be input as an analytical function. The user is given the choice of a linear function, "Corey's curves", "Grant's curves", Fatt and Kilikoff functions, Sandia functions, or Verma functions. Capillary pressure functions must also be input as analytical functions. The user may specify a linear function, Milly's function, Leverett's function, or the Sandia function.

References:

Pruess, K., 1984. TOUGH - A Numerical Model for Strongly Heat Driven Flow in Partially Saturated Media. LBL Earth Sciences Div. Annual Rept., Lawrence Berkeley Laboratory, Univ. of Calif., Berkeley, Calif., pp. 39-41.

Pruess, K., Y.W. Tsang, and J.S.Y. Wang. 1984. Modeling of Strongly Heat Driven Flow in Partially Saturated Fractured Porous Media. LBL-18552, Lawrence Berkeley Laboratory, Univ. of Calif., Berkeley, Calif.

Pruess, K. and J.S.Y. Wang, 1984. TOUGH - A Numerical Model for Nonisothermal Unsaturated Flow to Study Waste Canister Heating Effects. In: G.L. McVay (ed.) Mat. Res. Soc. Symp. Proc., Scientific Basis for Nuclear Waste Management, North Holland, New York, Vol. 26, pp. 1031-1038.

Pruess, K, Y.W. Tsang, and J.S.Y. Wang. 1984. Modeling of Strongly Heat-Driven Flow in Partially Saturated Fractured Porous Media. LBL-17490, Lawrence Berkeley Laboratory, Univ. of Calif., Berkeley, Calif.

Pruess, K. 1987. TOUGH User's Guide. NUREG/CR-4645, U.S. Nuclear Regulatory Commission, Washington, D.C.

Pruess, K. 1986. TOUGH--Users Guide. LBL-20700, Lawrence Berkeley Laboratory, Univ. of Calif., Berkeley, Calif.

Pruess, K. 1983. GMINC-- A Mesh Generator for Flow Simulations in Fractured Reservoirs. LBL-15227, Lawrence Berkeley Laboratory, Univ. of Calif., Berkeley, Calif.

Niemi, A., and G.S. Bodvarsson. 1988. Preliminary Capillary Hysteresis Simulations in Fractured Rocks, Yucca Mountain, Nevada. Journ. of Contaminant Hydrol., Vol. 3, pp. 277-291.

IGWMC Key: 2950 Model Name: TRANS

Authors: Walker, W.R., J.D. Sabey, and D.R. Hampton

Institution of Model Development: Colorado State University
Fort Collins, Colorado

Code Custodian: Hampton, D.R., Western Michigan University
Geology Department, Kalamazoo, MI 49008

Abstract:

TRANS is a finite element model for transient simulation of two-dimensional, horizontal, cross-sectional,or axial symmetric, coupled flow of heat and moisture in partially or fully saturated porous media, especially for assessment of buried thermal reservoirs and the heat exchange piping internal to the reservoirs.

Model developed for: research (e.g. hypothesis/theory testing)
Documentation includes: model theory, user's instructions
Availability: public domain

References:

Walker, W.R., J.D. Sabey and D.R. Hampton. 1981. Studies of Heat Transfer and Water Migration in Soils. Rept. Solar Energy Lab., Dept of Agri. and Chem. Eng., Colorado State University, Fort Collins, Colorado.

IGWMC Key: 3375 Model Name: MATTUM
Authors: Yeh, G.T. and R.J. Luxmoore
Institution of Model Development: Oak Ridge National Laboratory
Oak Ridge, Tennessee
Code Custodian: Yeh, G.T.
Penn State University, Dept. of Civil Eng.
225 Sackett Bldg, University Park, PA 16802

Abstract:

MATTUM is a three-dimensional model for simulating moisture and thermal transport in unsaturated porous media. The model solves both the flow equation and the heat transport equation under unsaturated water conditions using the integrated compartment method. The entire unsaturated zone is divided in a number of compartment of different sizes and shapes. The Philip-de Vries equations governing moisture movement and heat transfer are integrated over each of the compartments to yield a system of nonlinear ordinary differential equations. There three optional time integration schemes: split explicit, implicit pointwise iteration, and matrix inversion iteration.

Model developed for: research (e.g. hypothesis/theory testing), general use (e.g. in field applications)
Documentation includes: model theory, user's instructions, example problems, code listing, verification/validation
Verification/validation: verification (analyt.solutions)
Peer (independent) review: concepts, theory (math)

References:

Yeh, G.T. and R.J. Luxmoore. 1983. MATTUM: A Multidimensional Model for Simulating Moisture and Thermal Transport in Unsaturated Porous Media. ORNL-5888, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

IGWMC Key: 3590 Model Name: SPLASHWATER
Author: Milly, P.
Institution of Model Development: Princeton University, Water Resources Program
Dept. of Civil Engineering, Princeton, NJ 08544
Code Custodian: Milly, P.C.D.
Princeton University, Dept. of Civil Engineering
Princeton, NJ 08544

Abstract:

SPLASHWATER is a finite element model for simulation of coupled heat and moisture fields in the unsaturated zone. The model includes evapotranspiration, hysteresis, and heat convection and conduction.

Model developed for: research (e.g. hypothesis/theory testing)
Documentation includes: model theory, user's instructions, example problems, code listing, verification/validation
Verification/validation: verification (analyt.solutions)
Availability: restricted public domain

References:

Milly, P.C.D. 1982. Moisture and Heat Transport in Hysteretic, Inhomogeneous Porous Media: A Matric Head-Based Formulation and Numerical Model. Water Resourc. Res., Vol. 18(3), pp. 489-498.

Milly, P.C.D. and P.S. Eagleson. 1980. The Coupled Transport of Water and Heat in a Vertical Soil Column Under Atmospheric Excitation. MIT Report No. 258, Massachusetts Inst. of Technology, Cambridge, Mass.

IGWMC Key: 5660 Model Name: FLASH

Authors: Baca, R.G., and S.O. Magnuson

Institution of Model Development: Idaho National Engineering Laboratory
EG&G, Inc., P.O. Box 1625, Idaho Falls, Idaho 83415

Code Custodian: Baca, R.G.
Idaho National Engineering Laboratory
Subsurface and Environm. Modeling Unit, Geoscience Group,
EG&G, Inc, P.O. Box 1625, Idaho Falls, Idaho 83415.

Abstract:

FLASH is a finite element model for simulation of two-dimensional, cross-sectional, variably saturated fluid flow in fractured porous media at an arid site, together with two-dimensional, horizontal, saturated flow in an underlying unconfined aquifer. In addition, the code has the capability to simulate heat conduction in the vadose zone. The Richard's equation for variably saturated flow is solved iteratively using a Picard or Newton iteration technique, the unconfined flow equation is solved using Newton-Raphson iteration. The variably saturated module handles 1st, 2nd and 3rd type b.c.'s, the saturated module only 1st and 2nd type b.c.'s. The FLASH code can be interfaced with the FLAME code to simulate contaminant transport in the subsurface.

Model developed for:	general use (e.g. in field applications)
Documentation includes:	model theory, user's instructions, example problems, program structure and development, verification/validation
Verification/validation:	verification (analyt.solutions), code intercomparison
Peer (independent) review:	concepts, theory (math)
Availability:	public domain

Remarks:

The FLASH and FLAME codes are extensions and refinements of the MAGNUM fluid flow code and the CHAINT contaminant transport code, respectively.

References:

Baca, R.G., and S.O. Magnuson. 1992. FLASH - A Finite Element Computer Code for Variably Saturated Flow. EGG-GEO-10274, Idaho National Engineering Laboratory, Idaho Falls, Idaho.

Appendix 6: Flow, Solute Transport and Heat Transport in the Unsaturated Zone

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IGWMC Key: 3234 Model Name: VADOSE
Authors: Sagar, B.
Institution of Model Development: Analytic & Computational Research,Inc.
Los Angeles, California
Code Custodian: B. Sagar
Southwest Research Inst., Div. 20
6220 Culebra Road, P.O. Drawer 0510
San Antonio, TX 38510
Abstract:

VADOSE is an integrated finite difference model for analysis of steady or transient, two-dimensional areal, cross-sectional or radial simulation of coupled density-dependent transport of moisture, heat and solutes in variably-saturated, heterogeneous, anisotropic porous media.

Model developed for: research (e.g. hypothesis/theory testing)
Documentation includes: model theory, user's instructions, example problems
Availability: proprietary, license

IGWMC Key: 3235 Model Name: FLOTRA
Authors: Sagar, B.
Institution of Model Development: Analytic & Computational Research, Inc.
Los Angeles, California
Code Custodian: B. Sagar
Southwest Research Inst., Div. 20
6220 Culebra Road, P.O. Drawer 0510
San Antonio, TX 38510
Abstract:

FLOTRA is an integrated finite difference model for simulation of steady or transient, two-dimensional areal, cross-sectional or radial, density- dependent flow, heat and mass transport in variably saturated, anisotropic, heterogeneous, deformable porous media.

Model developed for: research (e.g. hypothesis/theory testing), general use (e.g. in field applications)
Documentation includes: model theory, user's instructions, example problems
Availability: proprietary, license

IGWMC Key: 3830 Model Name: SUTRA
Authors: Voss, C.I.
Institution of Model Development: U.S. Geological Survey
Water Resources Div., National Center
Reston, Virginia
Code Custodian: Voss, C.I.
U.S. Geological Survey, 431 National Center, Reston, VA 22092
Abstract:

SUTRA (Saturated-Unsaturated TRAnsport) simulates transient or steady-state, two-dimensional, variably saturated, fluid density dependent ground water flow with transport of energy or chemically reactive species solute transport. The model employs a hybrid finite-element and integrated-finite-difference method to approximate the coupled equations. Solute transport include advection, dispersion, diffusion, equilibrium adsorption on the porous matrix, and both first-order and zero-order decay or production. Energy transport may take place in both the solid matrix and the liquid phase. SUTRA may be employed in both areal (horizontal) and cross-sectional mode for saturated systems or in cross-sectional mode only for unsaturated systems. (see remarks).

Model developed for:	research (e.g. hypothesis/theory testing), general use (e.g. in field applications), demonstration/education
Documentation includes:	model theory, user's instructions, example problems, program structure and development, code listing, verification/validation
Verification/validation:	verification (analyt.solutions), laboratory data sets
Peer (independent) review:	concepts, theory (math), documentation
Availability:	public domain, proprietary, purchase

Remarks:

SUTRA provides, as preliminary calculated results, fluid pressures and either solute concentrations or temperatures. Mesh construction is flexible for arbitrary geometries employing quadrilateral finite elements in Cartesian or radial-cylindrical coordinates. The mesh might be coarsened through the use of pinch nodes. Boundary conditions, sources and sinks may be time dependent. The model has a rest art option. Options are also available to print fluid velocities, and fluid mass, and solute mass or energy budgets for the system. SUTRA's numerical algorithms are not specifically applicable to non-linearities of unsaturated flow. Therefor SUTRA, as distributed by the USGS, requires fine spatial and temporal discretization for unsaturated flow. The user can replace the included function for unsaturated flow by others, and recompile the code.

An extension of the code SUTRA is the code SATRA-CHEM by Lewis (1984; 1986; see IGWMC Key # 3831). It includes sorption, ion exchange and equilibrium chemistry. The nonlinear components resulting from these chemical processes are reduced into two time-dependent variables that essentially plug into a general form of the classic advection-dispersion equation.

A main-frame version of SUTRA and an extended memory IBM PC-386 version is available from the International Ground Water Modeling Center, Colorado School of Mines, Golden, CO 80401.

An IBM PC/386 extended memory version of this model is also available from Geraghty & Miller, Inc., Modeling Group, 10700 Parkridge Blvd, # 600, Reston, VA 22091.

The new version of SUTRA (USGS, June 1990) includes a post-processor SUTRAPLOT, based on an contouring algorithm developed by Arlen Harbough.

References:

Voss, C.I. 1984. SUTRA: A Finite Element Simulation Model for Saturated-Unsaturated Fluid Density-Dependent Ground Water Flow with Energy Transport or Chemically Reactive Single Species Solute Transport. Water-Resources Investigations Report 84-4369, U.S. Geological Survey, Reston, Virginia.

Souza, W.R. 1987. Documentation of a Graphical Display Program for SUTRA Finite-Element Simulation Model. Water-Resources Investigations Report 87-4245, U.S. Geological Survey, Washington, D.C.

Wagner, J., and Ruiz-Calzada, C.E., (Date Unknown). Evaluation of Models for Unsaturated - Saturated Flow and Solute Transport. Cooperative agreement CR 81114-01-2 with Robert S. Kerr Environmental Research Laboratory and the School of Chemical Engineering, Oklahoma State University, Sillwater, OK.

IGWMC Key: 4550 Model Name: MOTIF (Model of Transport in Fractured/Porous Media)

Authors: Guvanasen, V.
Institution of Model Development: Atomic Energy of Canada, Ltd.
Whiteshell Nuclear Research Establishment
Pinawa, Manitoba, Canada

Code Custodian: Tin Chan
Atomic Energy of Canada, Ltd.
Whiteshell Nuclear Research Estb.
Pinawa, Manitoba, Canada R0E1I0

Abstract:

MOTIF is a finite element model to simulate one-, two-, and three-dimensional coupled processes of saturated or unsaturated fluid flow, conductive and convective heat transport, brine transport and single species radionuclide transport in a compressible rock of low permeability intersected with a few major fractures. The model includes diffusion into the rock matrix.

Model developed for:	research (e.g. hypothesis/theory testing), general use (e.g. in field applications)
Documentation includes:	model theory, user's instructions, verification/validation
Verification/validation:	verification (analyt.solutions), code intercomparison
Availability:	proprietary, license

Remarks:

MOTIF is especially suitable for modeling fractured rock mass since the 4-noded planar elements can be used to simulate flow in arbitrarily oriented planar fractures or fracture zones in a 3D model.

The code has been verified among others by comparison with closed-form solutions in the HYDROCOIN project. (see Chanet Al. 1986). It has been subject to AECL's internal quality assurance.

References:

Chan, T., V. Guvanasen and J.A. Reid. 1985. Numerical Modelling of Coupled Fluid, Heat and Solute Transport in Deformable Fractured Rock. International Symposium on Coupled Processes Affecting the Performance of a Nuclear Waste Repository, Berkeley, September, 18-20, 1985. Lawrence Berkeley Laboratory, Univ. of Calif., Berkeley, Calif.

Chan, T., N.W. Scheier and J.A.K. Reid. 1986. Finite Element Thermohydrogeological Modeling for Canadian Nuclear Fuel Waste Management. Second International Conference on Radioactive Waste Management, Winnipeg, September 1986.

Davison, C.C. and V. Guvanasen, 1985. Hydrogeological Characterization Modelling and Monitoring of the Site of Canada's Underground Research Laboratory. In: Proceed. Hydrogeology of Rocks of Low Permeability, IAH 17th Internat. Congress, Tuscon, Arizona, January 7-11, 1985. Internat. Assoc. of Hydrogeologists.

Chan, T., V. Guvanasen and B. Nakka. 1986. Verification of the MOTIF Finite Element Code Using HYDROCOIN Level 1 Cases 1,2, and 4. Atomic Energy of Canada, Ltd., Pinawa, Manitoba.

Guvanasen, V. 1984. Development of a Finite Element Code and its Application to Geoscience Research. In: Proceedings 17th Information Meeting of the Nuclear Waste Management Program. Atomic Energy of Canada, Ltd., Technical Record TR-199, pp. 554-566.

Chan, T., V. Guvanasen, and J.A.V. Rein. 1987. Numerical Modeling of Coupled Fluid, Heat and Solute Transport in Deformable Fractured Rock. In: C.F. Tsang (ed.), Coupled Processes Associated with Nuclear Waste Repositories, pp. 605-625. Academic Press, Orlando, Florida.

Chan, T. 1989. An Overview of Groundwater Flow and Radionuclide Transport Modeling in the Canadian Nuclear Fuel Waste Management Program. In: B.E. Buxton (ed.), Geostatistical Sensitivity and Uncertainty Methods for Groundwater Flow and Radionuclide Transport Modeling, pp.39-62. Battelle Press, Battelle Memorial Institute, Columbus, Ohio.

IGWMC Key: 5031 Model Name: CTSPAC

Authors: Lindstrom, F.T., D.E. Cawlfield, and L. Boersma

Institution of Model Development: Oregon State University, Dept. of Soil Science
Corvallis, Oregon

Code Custodian: L. Boersma
Dept. of Soil Science, Oregon State University
Corvallis, OR 97331

Abstract:

CTSPAC is an one-dimensional numerical model that couples the flow of water and the transport of heat and solutes in layered soils with the uptake and transport of water and solutes in plants. Initial root distribution is specified. The rate of uptake is a function of the environmental conditions that determine the plant's transpiration rate. Water transport in the plant is based on water potential and pressure gradients according to Munch pressure flow hypothesis. The model was developed for assessing risks involved in the use of xenobiotic chemicals. It allows an evaluation of the rate of uptake of such chemicals from the soil solution and the accumulation in the various plant parts.

Model developed for:	research (e.g. hypothesis/theory testing), general use (e.g. in field applications)
Documentation includes:	model theory, user's instructions, example problems
Peer (independent) review:	concepts, theory (math)
Availability:	public domain

References:

Lindstrom, F.T., D.E. Cawlfield, and L. Boersma. 1988. CTSPAC: Mathematical Model for Coupled Transport of Water, Solutes, and Heat in the Soil-Plant-Atmosphere Continuum. EPA/600/3-88/030, U.S. Environmental Protection Agency, Environm. Research. Lab., Corvallis, Oregon.

Boersma, L., F.T. Lindstrom, C. McFarlane and E.L. McCoy. 1988. Model of Coupled Transport of Water and Solutes in Plants. Spec. Report No. 818. Agric. Experim. Station, Oregon State Univ., Corvallis, Oregon.

IGWMC Key: 3238 Model Name: PORFLOW-3D
Author: Runchal, A.K.
Institution of Model Development: Analytic and Computational Research, Inc., Bel Air, Calif.

Code Custodian: Akshai Runchal
1931 Stradella Road, Bel Air, CA 90077

Abstract:

PORFLOW-3D is an integrated finite difference model to simulate coupled transient or steady-state, multiphase, fluid flow, and heat, salinity, or chemical species transport in variably saturated porous or fractured, anisotropic and heterogeneous media. The program facilitates arbitrary sources or sinks in three-dimensional cartesian or axisymmetric (cylindrical) geometry. The user interface is based on the FREEFORM language using simple English-like commands. The software includes the ARCPLOT graphic post processor.

Model developed for:	research (e.g. hypothesis/theory testing), general use (e.g. in field applications), demonstration/education
Documentation includes:	model theory, user's instructions, example problems, verification/validation
Verification/validation:	verification (analyt.solutions)
Availability:	proprietary, license

Remarks:

PORFLOW II and PORFLOW III have been used extensively in real life problem solving. A version of this model is being used to simulate the near-field behavior of high level nuclear waste repository in basalt.

PORFLOW II and PORFLOW III provide optional coupling with thermo-mechanical stress model, developed by the same author. A version of the PORFLOW series, PORFLOW-R, provides special features for simulation of transport processes around high-level waste repositories. These include, for example, an option to calculate the instantaneous or cumulative nuclide flux crossing a given boundary.

See also PORFLO (IGWMC Key # 3790), PORFLOW-2D (IGWMC Key # 3233), and PORFLOW-3D (IGWMC Key # 3238).

References:

Runchal, A.K. 1982. PORFLOW-R: A Mathematical Model for Coupled Ground Water Flow, Heat Transfer and Radionuclide Transport in Porous Media. Techn. Rept. Rep-014, Analytic & Computational Research, Inc., West Los Angeles, California.

Runchal, A.K. 1981. PORFLOW-F: A Mathematical Model for Ground Water Flow with Heat Transfer, Freezing, Thawing and Atmospheric Heat Exchange, Volume I - Theory. Techn Report REP-006a, Analytic & Computational Research, Inc., West Los Angeles, California.

Runchal, A.K., and G. Hocking. 1981. An Equivalent Continuum Model for Fluid Flow, Heat and Mass Transport in Geological Materials. Paper 81-HT-54, ASME, 20th Joint ASME/AIChE National Heat Transfer Conference, Milwaukee, Wisconsin, August 2-5.

Runchal, A.K. 1982. Mathematical Basis of Porous Media Flow, Heat and Mass Transfer. Techn. Report REP-008, Analytic & Computational Research, Inc., West Los Angeles, Calif.

Runchal, A.K. 1982. The Density and Viscosity Relations for Water. Techn. Report REP-009, Analytic & Computational Research, Inc., West Los Angeles, Calif.

Runchal, A.K. 1987. Theory and Application of the PORFLOW Model for Analysis of Coupled Fluid Flow, Heat and Radionuclide Transport in Porous Media. In: C.-F. Tsang (ed.), Coupled Processes Associated with Nuclear Waste Repositories, Academic Press, New York, New York, pp. 495-516.

IGWMC Key: 5213 Model Name: TDFD1O (Two-Dimensional Finite Difference 1st Order sorption)
Authors: Slotta, L.S.
Institution of Model Development: Slotta Engineering Associates, Inc, Corvallis, Oregon

Code Custodian: Jalal Heydarpour
Slotta Engineering Associates, Inc.
P.O. Box 1376, Corvallis, OR 97339

Abstract:

TDFD1O is a two-dimensional model for simultaneous simulation of movement of moisture, transport of heat, and transport and fate of a contaminant in a shallow unconfined aquifer. The porous medium may be heterogeneous. The coupled system of non-linear unsaturated/saturated moisture flow and heat and chemical transport are solved using a finite difference approximation. The porous medium is partitioned in three fractions: sand, clay, and organic material, with for each fraction first-order sorption kinetics included. Time integration is performed using the backward Euler method. Dynamic boundary conditions at the air-porous medium interface are included. A variety of first- and second-type boundary conditions are included.

Model developed for: general use (e.g. in field applications)
Documentation includes: user's instructions, example problems

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IGWMC Key: 5860 Model Name: NEWTMC
Authors: Lindstrom, F.T. (1), and F.T. Piver, F.T.
Institution of Model Development: 1) Dept. of Math., Oregon State Univ., Corvallis;
2) Nat. Inst. of Health, Research Triangle Park, NC.

Code Custodian: Lindstrom, F.T.
Dept. of Mathematics, Oregon State Univ., Corvallis, OR 97331

Abstract:

NEWTMC is an one-dimensional mass balance model for simulating the transport and fate of nonionizable organic compounds in unsaturated/saturated porous media. Using the principles of water mass, momentum, heat energy and chemical mass balance, the model solves simultaneously for moisture, temperature and liquid phase chemical concentration. The model uses a dynamic free boundary to represent the air-soil interface and a prescribed water table height as lower boundary. The model allows for elaborate simulation of air conditions at the air-soil interface, allowing the boundary conditions to be dependent on the air conditions. Chemicals may be introduced via incoming air (vapor phase), rain water, inflow from the water table, or initially distributed within the soil column.

Model developed for: research (e.g. hypothesis/theory testing)
Documentation includes: model theory, user's instructions, example problems, verification/validation
Verification/validation: laboratory data sets
Peer (independent) review: concepts, theory (math)

Availability: public domain

References:

Lindstrom, F.T., and W.T. Piver. 1985. A Mathematical Model for the Transport and Fate of Organic Chemicals in Unsaturated/Saturated Soils. Environm. Health Perspectives, Vol. 60, pp. 11-28.

Lindstrom, F.T., and W.T. Piver. 1984. A Mathematical Model for Simulating the Fate of Toxic Chemicals in a Simple Terrestrial Microcosm. Techn. Rept. 51, Dept. of Math. and Stat., Oregon State Univ., Corvallis, Oregon.

Appendix 7: Parameter Estimation for Flow and Transport in the Unsaturated Zone

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IGWMC Key: 3433 Model Name: ONESTEP
Authors: Kool, J.B., J.C. Parker, and M.Th. Van Genuchten.
Institution of Model Development: Virginia Polytechn. Inst.
Blacksburg, Virginia
Code Custodian: J.C. Parker
Virginia Polytechn. Inst.
245 Smyth Hall, Blacksburg, VA 24061

Abstract:

ONESTEP is a nonlinear parameter estimation model for evaluating soil hydraulic properties from one-step outflow experiments in the one-dimensional flow. The program estimates parameters in the van Genuchten soil hydraulic property model from measurements of cumulative outflow with time during one-step experiments. The program combines non-linear optimization with a Galerkin finite element model.

Model developed for:	research (e.g. hypothesis/theory testing), demonstration/education
Documentation includes:	model theory, user's instructions, example problems, verification/validation
Verification/validation:	verification (analyt.solutions), laboratory data sets
Peer (independent) review:	concepts, theory (math)
Availability:	proprietary, purchase

Remarks:

An IBM-PC version is available from the International Ground Water Modeling Center, Colorado School of Mines, Golden, CO 80401.

References:

Kool, J.B., J.C. Parker, and M.Th. Van Genuchten. 1985. ONESTEP: A Nonlinear Parameter Estimation Program for Evaluating Soil Hydraulic Properties from One-Step Outflow Experiments. Bulletin 85-3, Virginia Polytechn. Inst., Blacksburg, Virginia.

IGWMC Key: 6330 Model Name: SOIL
Authors: El-Kadi, A.I.
Institution of Model Development: International Ground Water Modeling Center
Holcomb Research Institute, Indianapolis, Indiana
Code Custodian: International Ground Water Modeling Center
Colorado School of Mines, Golden, CO 80401

Abstract:

SOIL estimates the parameters of the soil hydraulic functions. For the soil-water characteristic function the user can choose from the methods of Brooks and Corey (1964), Brutsaert (1966), Vauclin et al. (1979), and van Genuchten (1978). The parameters for the chosen function are obtained using non-linear least-squares analysis. The unsaturated hydraulic conductivity function is estimated by the series-parallel model of Childs and Collis-George (1950) and is obtained by straight-line fitting on a log-log curve. With the derived parameters, the program computes for selected pressures the observed and fitted moisture contents and the soil hydraulic properties. The results are plotted graphically on screen. If saturated hydraulic conductivity is unknown the program provides an estimated value. The menu-driven, user-interactive code requires as input pairs of measured water content and suction, and the saturated water content that corresponds with zero suction.

Model developed for: general use (e.g. in field applications)
Documentation includes: model theory, user's instructions, example problems, code listing
Availability: public domain

References:

El-Kadi, A.I. 1987. Estimating the Parameters of Soil Hydraulic Properties SOIL, Microcomputer Interactive Version. BAS-14, Internat. Ground Water Modeling Center, Holcomb Research Inst., Indianapolis, Indiana.

El-Kadi, A.I. 1984. Automated Estimation of the Parameters of Soil Hydraulic Properties. GWMI 84-12, Internat. Ground Water Modeling Center, Holcomb Research Inst., Indianapolis, Indiana.

IGWMC Key: 6170 Model Name: FP
Authors: Su, C., and R.H. Brooks
Institution of Model Development: Oregon State University, Dept. of Agricultural Eng., Corvallis, Oregon
Code Custodian: Dept. of Agricultural Eng., Oregon State University Corvallis, OR 97331

Abstract:

FP is a program to determine the parameters of the retention function (the soil-water characteristic function) from experimental data. Based upon the Pearson Type VIII distribution function, a general retention function which relates the saturation to the capillary pressure in distributed soils has been formulated. This simple, yet complete function has been shown to describe the imbibition as well as the drainage branch of the retention curve. It is defined by four readily assessed parameters that either have physical significance themselves or may be used to determine some hydraulic properties of the soil. Please see "Remarks" for more information.

Model developed for: research (e.g. hypothesis/theory testing), general use (e.g. in field applications)
Documentation includes: model theory, user's instructions, example problems
Availability: public domain

Remarks:

With the assumption that the Burdine integrals are adequate, a relative permeability function has been derived through the substitution of the retention function for the integrands in the Burdine Integrals. The permeability function is expressed in terms of the incomplete Beta function ration whose value may be conveniently found in some mathematical tables.

A general pore-sized distribution function of soils has been obtained from the retention function. The derivation of the pore-size distribution function enables more rigorous examination and further exploration of the theories concerning water movement in partially saturated soils. In this respect, an explanation of the phenomenon of air entrapment during imbibition has been offered through an energy concept based upon the pore-size distribution function along with the retention function. Two criteria of affinity have been established for porous media. Media are said to be affine if their corresponding pore-size distribution parameters are identical. The scaling factor for the external dimension of the model has been chosen to be the capillary pressure head at the inflection point of the retention curve, whose value is always finite. The analysis of the effect of the pore-size distribution parameters upon the retention, permeability, and diffusivity curves shows that the parameter governing the downward concavity of the retention curve is as important as that

governing the upward concavity when it comes to computing the permeability values from the retention data.

This model is available from the International Ground Water Modeling Center, Colorado School of Mines, Golden, CO 80401.

References:

Su, C., and R.H. Brooks. 1976. Hydraulic Functions of Soils from Physical Experiments. WRRI-41, Dept. of Agricultural Eng., Oregon State Univ., Corvallis, Oregon.

IGWMC Key: 6226 Model Name: SOHYP

Authors: Van Genuchten, M. Th.
Institution of Model Development: Princeton University, Dept. of Civil Eng.
Princeton, New Jersey
Code Custodian: M.Th. van Genuchten
USDA Salinity Laboratory, 4500 Glenwood Drive, Riverside, CA 92501

Abstract:

SOHYP is an analytical model for calculation of the unsaturated hydraulic conductivity function using soil moisture retention data. The basis of SOHYP is a relatively simple equation for soil moisture content-pressure head curve. The particular form of the equation enables one to derive closed-form analytical expressions for the relative hydraulic conductivity, when substituted in the predictive conductivity models of Burdine or Mualem. The resulting expressions for the hydraulic conductivity as function of the pressure head contain three independent parameters which may be obtained by fitting the described soil moisture retention model to experimental soil moisture retention data. The solution is based on automatic curve-fitting using a nonlinear least squares method.

Model developed for: research (e.g. hypothesis/theory testing), general use (e.g. in field applications)
Documentation includes: model theory, user's instructions
Availability: public domain

Remarks:

This model is available from the International Ground Water Modeling Center, Colorado School of Mines, Golden, CO 80401.

References:

Van Genuchten, M.Th. 1978. Calculating the Unsaturated Hydraulic Conductivity with a New Closed-form Analytical Model. 78-WR-08, Water Resources Program, Princeton University, Princeton, New Jersey.

IGWMC Key: 5183 Model Name: SOILPROP

Authors: Mishra, S., J.C. Parker, and N. Singhal
Institution of Model Development: Environmental Systems & Technologies, Inc.
Blacksburg, Virginia
Code Custodian: J.C. Parker
Environmental Systems & Technologies, Inc.
P.O. Box 10547, Blacksburg, VA 24062-0457

Abstract:

SOILPROP is an interactive program to estimate soil hydraulic properties and their uncertainty from particle size distribution data. Properties estimated by the program are the saturated hydraulic conductivity and parameters in the van Genuchten and Brooks-Corey models which describe the relationship between soil water content, capillary pressure and relative permeability. SOILPROP is based on the premise that the soil-water retention function reflects a pore size distribution which in turn can be inferred from the grain size distribution. The Arya-Paris procedure is used to compute theoretical water content versus capillary pressure curve, which is then fitted to the two models. Covariances are estimated using a first-order error analysis procedure.

Model developed for:	research (e.g. hypothesis/theory testing), general use (e.g. in field applications), demonstration/education
Documentation includes:	model theory, user's instructions, example problems, verification/validation
Verification/validation:	verification (analyt.solutions)
Peer (independent) review:	concepts, theory (math)
Availability:	proprietary, license

Remarks:

The saturated hydraulic conductivity in SOILPROP is estimated from the user-specified porosity and grain-size distribution data using a Kozeny-Carmen type equation.

References:

Arya, L.M., and J.F. Paris. 1981. A Physico-Empirical Model to Predict Soil Moisture Characteristics from Particle Size Distribution and Bulk Density Data. Soil Sci. Soc. Amer. Journ., Vol. 45, pp. 1023-1030.

Mishra, S.J., J.C. Parker, and N. Singhal. 1989. Estimation of Soil Hydraulic Properties and their Uncertainty from Particle Size Distribution Data. Journ. of Hydrology, Vol. 108, pp. 1-18.

Mishra, S., and J.C. Parker. 1989. Effects of Parameter Uncertainty on Prediction of Unsaturated Flow. Journ. of Hydrology, Vol. 108, pp. 19-33.

IGWMC Key: 5187 Model Name: FLOFIT

Authors: Kool, J.B., S. Mishra, and J.C. Parker

Institution of Model Development: Environmental Systems & Technologies, Inc., Blacksburg, Virginia

Code Custodian: J.C. Parker
Environmental Systems & Technologies, Inc.
P.O. Box 10457, Blacksburg, VA 24062-0457

Abstract:

FLOFIT is a program to estimate unsaturated soil hydraulic properties and/or transport parameters from 1-dimensional vertical flow/transport experiments. Three modes of operation are possible: 1) flow properties may be estimated from transient flow data; 2) solute dispersion and linear adsorption parameters may be estimated from steady flow transport data; or 3) flow and transport parameters may be estimated simultaneously from transient unsaturated flow and tracer experiments. Hydraulic properties are described by a hysteric van Genuchten model and dispersion by a scale-dependent function. Hydraulic and/or transport parameters may differ between layers. Numerical inversion of governing equations is performed using an efficient Levensberg-Marquardt algorithm.

Model developed for:	research (e.g. hypothesis/theory testing), general use (e.g. in field applications)
Documentation includes:	user's instructions
Availability:	proprietary, license

IGWMC Key: 6228 Model Name: RETC (Retention Curve Computer Code)
Authors: Van Genuchten, M.Th., F.J. Leij, and S.R. Yates
Institution of Model Development: USDA Salinity Lab., Riverside, California

Code Custodian: M.Th. van Genuchten
U.S. Dept. of Agriculture, U.S. Salinity Lab., Agric. Res. Service, 4500 Glenwood Drive, Riverside, Calif. 92501

Abstract:

RETC uses theoretical methods to predict the soil water retention curve and the hydraulic conductivity curve from measured soil water retention data. It uses several analytical models to estimate water retention, unsaturated hydraulic conductivity or soil water diffusivity for a given soil. It includes the parametric equations of Brooks-Corey and van Genuchten, which are used in conjunction with the theoretical pore-size distribution models of Mualem and Burdine to predict unsaturated hydraulic conductivity from observed soil water retention data. RTC can be used in a forward mode and in a parameter fitting mode. In the forward mode it estimates the soil-water retention curve and hydraulic conductivity; in the parameter fitting mode it determines the analytical model parameters.

Model developed for:	general use (e.g. in field applications), demonstration/education
Documentation includes:	model theory, user's instructions, example problems, program structure and development, code listing, verification/validation
Verification/validation:	verification (analyt.solutions), laboratory data sets, field datasets (validation)
Peer (independent) review:	concepts, theory (math), documentation
Availability:	public domain

Remarks:

This software is available from the Center for Subsurface Modeling Support (CSMOS), R.S. Kerr Environmental Research Laboratory, U.S. Environmental Protection Agency, P.O. Box 1198, Ada, OK 74820

References:

van Genuchten, M.Th., F.J. Leij and S.R. Yates. 1991. The RETC Code for Quantifying the Hydraulic Functions of Unsaturated Soils. EPA/600/2-91/065, U.S. Environm. Protection Agency, R.S. Kerr Environm. Res. Lab., Ada, Oklahoma.

Appendix 8: List of Input Requirements for Selected Unsaturated Zone Models

RITZ

Fractional organic carbon content
Soil bulk density
Saturated water content of soil
Saturated hydraulic conductivity
Clapp and Hornberger constant
Concentration of pollutant in sludge
Organic carbon partition coefficient
Oil-water partition coefficient
Henry's law constant
Diffusion constant of pollutant in air
Half life of pollutant
Concentration of oil in sludge
Density of oil
Half life of oil
Sludge application rate
Plow zone depth
Treatment zone depth
Recharge rate
Evaporation rate
Air temperature
Relative humidity
Diffusion coefficient of water vapor in air

FLAME

Control
- Type of transport simulation (time-varying or steady-state)
- Characteristics of boundary value problem (uniform or non-uniform initial condition; specified boundary conditions; point sources)
- Computational solution procedures (band or frontal solver; linear or quadratic finite element shape functions)
- Coordinate system to be used (cartesian or radial; vertical, horizontal or planar)
- Output print control (echo all; minimum echo; full echo)
- File input control (files for mesh, initial conditions, soil properties, head, velocity, restart, and/or) results
- Planes for which mass flux across is to be calculated
- Time integration factor
- Minimum change in concentration
- Maximum change in concentration
- Grid scale factor in x- and y-direction
- Time dependent data (number of subintervals; output time plane for each subinterval)

Nodal and element data
- Grid information (element number, corresponding node numbers, element material number, element ordering index; node number, x-coordinate and z-coordinate)
- Initial conditions (location and value)
- Boundary conditions (location type and value: fixed concentration for 1st type; time of application/duration and mass source rate for 2nd type)

Material data
- Element data (material number, longitudinal and transverse dispersivity, saturated hydraulic conductivity in x- and z-direction, saturated moisture content or porosity, line element width, retardation factor, half-life, molecular diffusion coefficient, tortuosity in x- and z-direction)
- Characteristic and relative hydraulic conductivity curve data (tabular data including pressure heads, volumetric moisture content, relative hydraulic conductivity)

Control

- Processes to be modelled (heat transport, unsaturated flow, Dupuit-Forcheimer flow, horizontal flow)
- Type of simulation (time-varying or steady-state)
- Characteristics of boundary value problem (uniform or non-uniform initial condition; specified boundary conditions, constant or time-varying flux, or mixed boundary condition)
- Computational solution procedures (Picard or Newton iteration; band or frontal solver; linear or quadratic finite element shape functions)
- Coordinate system to be used (cartesian or radial; vertical, horizontal or planar)
- Output print control (echo all; minimum echo; full echo)
- File input control (files for mesh, initial conditions, soil properties, head, velocity, restart, and/or) results
- Planes for which mass flux across is to be calculated
- Time integration factor
- Relative error criteria
- Maximum change in pressure head
- Maximum change in temperature
- Grid scale factor in x- and y-direction
- Time dependent data (number of subintervals; output time plane for each subinterval)

Nodal and element data

- Grid information (element number, corresponding node numbers, element material number, element ordering index; node number, x-coordinate and z-coordinate)
- Initial conditions (location and value for pressure head or temperature)
- Boundary conditions (location type and value: transient fixed pressure head for unsaturated flow or total head for saturated flow for 1st type; transient volumetric heat or fluid flux for 2nd type)

Material data

- Element data (material number, volumetric heat capacity, thermal conductivity, specific storage, saturated conductivity in x- and z-direction, saturated moisture content or porosity, line element width)
- Characteristic and relative hydraulic conductivity curve data (tabular data including pressure heads, volumetric moisture content, relative hydraulic conductivity)
- Relationship of thermal conductivity and moisture content or pressure head (tabular data)

Unsaturated zone

Saturated hydraulic conductivity
Unsaturated zone porosity
Air entry pressure head
Depth of unsaturated zone
Number of nodal points residual water content
Number of porous materials
Number of layers
Alfa coefficient
Van Genuchten exponent
Thickness of each layer
Longitudinal dispersivity of each layer
Percent organic matter
Bulk density of soil for each layer
Biological decay coefficient for unsaturated zone

Acid catalyzed hydrolysis rate
Neutral hydrolysis rate constant
Base catalyzed hydrolysis rate
Reference temperature
Normalized distribution coefficient
Air diffusion coefficient
Reference temperature for air diffusion
Molecular weight
Infiltration rate
Area of waste disposal unit
Duration of pulse
Source decay constant
Initial concentration at landfill
Particle diameter

Saturated zone

Recharge rate
Overall 1st order decay for saturated zone
Biodegradation coefficient for saturated zone
Aquifer thickness
Hydraulic gradient
Longitudinal dispersivity
Transverse dispersivity

Vertical dispersivity
Temperature of aquifer
pH
Organic carbon content
Well distance from site
Angle off center
Well vertical distance

Variable	Definition
DX1(NN)	XX Component of hydrodynamic dispersion tensor at left side of cell times $\Delta x/\Delta z$, L^2T^{-1}.
DX2(NN)	XZ Component of hydrodynamic dispersion tensor at left side of cell times $\Delta x/2\Delta z$, L^2T^{-1}.
DZ1(NN)	ZZ Component of hydrodynamic dispersion tensor at top of cell times $\Delta z/\Delta x$, L^2T^{-1}.
DZ2(NN)	ZX Component of hydrodynamic dispersion tensor at top of cell times $\Delta z/2\Delta x$, L^2T^{-1}.
VX(NN)	X Velocity at left side of cell, LT^{-1}.
VZ(NN)	Z Velocity at top of cell, LT^{-1}.
CC(NN)	Concentration, ML^{-3}.
COLD(NN)	Concentration at previous time step, ML^{-3}.
CS(NN)	Concentration of specified fluid sources, ML^{-3}.
QT(NN)	Fluid flux through constant head nodes, L^3T^{-1}.
NCTYP(NN)	Boundary condition or cell type indicator: 0 = internal node, 1 = specified concentration node, and 2 = specified solute flux node.
RET(NN)	Slope of adsorption isotherm times bulk density, dimensionless.
ANG	Angle at which grid is to be tilted, degrees.
TRANS	If = T, solute transport and flow are to be simulated; if = F, only flow is simulated.
TRANS1	If = T, matrix solver solves for head; if = F, matrix solver solves for concentration.
SSTATE	If = T, steady-state flow has been achieved.
CIS	If = T, centered-in-space differencing is used for transport equation; if = F, backward-in-space differencing is used.
CIT	If = T, centered-in-time differencing is used for transport equation; if = F, backward-in-time differencing is used.
EPS1	Convergence criteria for transport equation, ML^{-3}.
VPNT	If = T, velocities are written to file 6.
SORP	If = T, nonlinear sorption is to be simulated.

Note: NN = number of nodes

Card	Variable	Description
		[Line group A read by VSEXEC]
A-1	TITL	80-character problem description (formatted read, 20A4).
A-2	TMAX	Maximum simulation time, T.
	STIM	Initial time (usually set to 0), T.
	ANG	Angle by which grid is to be tilted (Must be between -90 and +90 degrees, ANG = 0 for no tilting, see Supplemental Information for further discussion), degrees.
A-3	ZUNIT	Units used for length (A4).
	TUNIT	Units used for time (A4).
	CUNX	Units used for mass (A4).
Note: Line A-3 is read in 3A4 format, so the unit designations must occur in columns 1-4, 5-8, 9-12, respectively.		
A-4	NXR	Number of cells in horizontal or radial direction.
	NLY	Number of cells in vertical direction.
A-5	NRECH	Number of recharge periods.
	NUMT	Maximum number of time steps.
A-6	RAD	Logical variable = T if radial coordinates are used; otherwise = F.
	ITSTOP	Logical variable = T if simulation is to terminate after ITMAX iterations in one time step; otherwise = F.
	TRANS	Logical variable = T if solute transport is to be simulated.
Line A-6A is present only if TRANS = T.		
A-6A	CIS	Logical variable = T if centered-in-space differencing is to be used; = F if backward-in-space differencing is to be used for transport equation.
	CIT	Logical variable = T if centered-in-time differencing is to be used; = F if backward-in-time or fully implicit differencing is to be used.
	SORP	Logical variable = T if nonlinear sorption or ion exchange is to be simulated. Nonlinear sorption occurs when ion exchange, Langmuir isotherms, or Freundlich isotherms with n not equal to 1 are used.
A-7	F11P	Logical variable = T if head, moisture content, and saturation at selected observation points are to be written to file 11 at end of each time step; otherwise = F.

Card	Variable	Description
A-7--Continued	F7P	Logical variable = T if head changes for each iteration in every time step are to be written in file 7; otherwise = F.
	F8P	Logical variable = T if output of pressure heads (and concentrations if TRANS = T) to file 8 is desired at selected observation times; otherwise = F.
	F9P	Logical variable = T if one-line mass balance summary for each time step to be written to file 9; otherwise = F.
	F6P	Logical variable = T if mass balance is to be written to file 6 for each time step; = F if mass balance is to be written to file 6 only at observation times and ends of recharge periods.
A-8	THPT	Logical variable = T if volumetric moisture contents are to be written to file 6; otherwise = F.
	SPNT	Logical variable = T if saturations are to be written to file 6; otherwise = F.
	PPNT	Logical variable = T if pressure heads are to be written to file 6; otherwise = F.
	HPNT	Logical variable = T if total heads are to be written to file 6; otherwise = F.
	VPNT	Logical variable = T if velocities are to be written to file 6; requires TRANS = T.
A-9	IFAC	= 0 if grid spacing in horizontal (or radial) direction is to be read in for each column and multiplied by FACX. = 1 if all horizontal grid spacing is to be constant and equal to FACX. = 2 if horizontal grid spacing is variable, with spacing for the first two columns equal to FACX and the spacing for each subsequent column equal to XMULT times the spacing of the previous column, until the spacing equals XMAX, whereupon spacing becomes constant at XMAX.

Card	Variable	Description
A-9--Continued	FACX	Constant grid spacing in horizontal (or radial) direction (if IFAC=1); constant multiplier for all spacing (if IFAC=0); or initial spacing (if IFAC=2), L.
Line set A-10 is present if IFAC = 0 or 2.		
If IFAC = 0,		
A-10	DXR	Grid spacing in horizontal or radial direction. Number of entries must equal NXR, L.
If IFAC = 2,		
A-10	XMULT	Multiplier by which the width of each node is increased from that of the previous node.
	XMAX	Maximum allowed horizontal or radial spacing, L.
A-11	JFAC	= 0 if grid spacing in vertical direction is to be read in for each row and multiplied by FACZ. = 1 if all vertical grid spacing is to be constant and equal to FACZ. = 2 if vertical grid spacing is variable, with spacing for the first two rows equal to FACZ and the spacing for each subsequent row equal to ZMULT times the spacing at the previous row, until spacing equals ZMAX, whereupon spacing becomes constant at ZMAX.
	FACZ	Constant grid spacing in vertical direction (if JFAC=1); constant multiplier for all spacing (if JFAC =0); or initial vertical spacing (if JFAC=2), L.
Line set A-12 is present only if JFAC = 0 or 2.		
If JFAC = 0,		
A-12	DELZ	Grid spacing in vertical direction; number of entries must equal NLY, L.
If JFAC = 2,		
A-12	ZMULT	Multiplier by which each node is increased from that of previous node.
	ZMAX	Maximum allowed vertical spacing, L.
Line sets A-13 to A-14 are present only if F8P = T,		
A-13	NPLT	Number of time steps to write heads and concentrations to file 8 and heads, concentrations, saturations, and/or moisture contents to file 6.

Card	Variable	Description
A-14	PLTIM	Elapsed times at which pressure heads and concentrations are to be written to file 8, and heads, concentrations, saturations, and/or moisture contents to file 6, T.
Line sets A-15 to A-16 are present only if F11P = T,		
A-15	NOBS	Number of observation points for which heads, concentrations, moisture contents, and saturations are to be written to file 11.
A-16	J,N	Row and column of observation points. A double entry is required for each observation point, resulting in 2xNOBS values.
Lines A-17 and A-18 are present only if F9P = T.		
A-17	NMB9	Total number of mass balance components to be written to File 9.
A-18	MB9	The index number of each mass balance component to be written to file 9. (See table 7 in Supplemental Information for index key)
	[Line group B read by subroutine VSREAD]	
B-1	EPS	Closure criteria for iterative solution of flow equation, units used for head, L.
	HMAX	Relaxation parameter for iterative solution. See discussion in Lappala and others (1987) for more detail. Value is generally in the range of 0.4 to 1.2.
	WUS	Weighting option for intercell relative hydraulic conductivity: WUS = 1 for full upstream weighting. WUS = 0.5 for arithmetic mean. WUS = 0.0 for geometric mean.
	EPS1	Closure criteria for iterative solution of transport equation, units used for concentration, ML^{-3}. Present only if TRANS = T.
B-3	MINIT	Minimum number of iterations per time step.
	ITMAX	Maximum number of iterations per time step. Must be less than 200.
B-4	PHRD	Logical variable = T if initial conditions are read in as pressure heads; = F if initial conditions are read in as moisture contents.

Card	Variable	Description
B-5	NTEX	Number of textural classes or lithologies having different values of hydraulic conductivity, specific storage, and/or constants in the functional relations among pressure head, relative conductivity, and moisture content.
	NPROP	Number of flow properties to be read in for each textural class. When using Brooks and Corey or van Genuchten functions, set NPROP = 6, and when using Haverkamp functions, set NPROP = 8. When using tabulated data, set NPROP = 6 plus number of data points in table. [For example, if the number of pressure heads in the table is equal to N1, then set NPROP =3*(N1+1)+3]
	NPROP1	Number of transport properties to be read in for each textural class. For no adsorption set NPROP1 = 6. For a Langmuir or Freundlich isotherm set NPROP1 = 7. For ion exchange set NPROP1 = 8. Present only if TRANS = T.
Line sets B-6, B-7, and B-7A must be repeated NTEX times		
B-6	ITEX	Index to textural class.
B-7	ANIZ(ITEX)	Ratio of hydraulic conductivity in the z-coordinate direction to that in the x-coordinate direction for textural class ITEX.
	HK(ITEX,1)	Saturated hydraulic conductivity (K) in the x-coordinate direction for class ITEX, LT^{-1}.
	HK(ITEX,2)	Specific storage (S_s) for class ITEX, L^{-1}.
	HK(ITEX,3)	Porosity for class ITEX.

Definitions for the remaining sequential values on this line are dependent upon which functional relation is selected to represent the nonlinear coefficients. Four different functional relations are allowed: (1) Brooks and Corey, (2) van Genuchten, (3) Haverkamp, and (4) tabular data. The choice of which of these to use is made when the computer program is compiled, by including only the function subroutine which pertains to the desired relation (see discussion in Lappala and others (1987) for more detail).

Card	Variable	Description
B-7--Continued		
In the following descriptions, definitions for the different functional relations are indexed by the above numbers. For tabular data, all pressure heads are input first (in decreasing order from the largest to the smallest), all relative hydraulic conductivities are then input in the same order, followed by all moisture contents.		
HK(ITEX,4)	(1)	h_b, L. (must be less than 0.0).
	(2)	α', L. (must be less than 0.0).
	(3)	A', L. (must be less than 0.0).
	(4)	Largest pressure head in table.
HK(ITEX,5)	(1)	Residual moisture content (θ_r).
	(2)	Residual moisture content (θ_r).
	(3)	Residual moisture content (θ_r).
	(4)	Second largest pressure head in table.
HK(ITEX,6)	(1)	λ, pore-size distribution index.
	(2)	β'.
	(3)	B'.
	(4)	Third largest pressure head in table.
HK(ITEX,7)	(1)	Not used.
	(2)	Not used.
	(3)	α, L. (must be less than 0.0).
	(4)	Fourth largest pressure head in table.
HK(ITEX,8)	(1)	Not used.
	(2)	Not used.
	(3)	β.
	(4)	Fifth largest pressure head in table.

For functional relations (1), (2), and (3) no further values are required on this line for this textural class. For tabular data (4), data input continues as follows:

HK(ITEX,9)	Next largest pressure head in table.
K(ITEX,N1+3)	Minimum pressure head in table. (Here N1 = Number of pressure heads in table; NPROP = 3*(N1+1)+3).
HK(ITEX,N1+4)	Always input a value of 99.
HK(ITEX,N1+5)	Relative hydraulic conductivity corresponding to first pressure head.
HK(ITEX,N1+6)	Relative hydraulic conductivity corresponding to second pressure head.
.	
.	
.	
HK(ITEX,2*N1+4)	Relative hydraulic conductivity corresponding to smallest pressure head.
HK(ITEX,2*N1+5)	Always input a value of 99.
HK(ITEX,2*N1+6)	Moisture content corresponding to first pressure head.

Card	Variable	Description
B-7--Continued		
HK(ITEX,2*N1+7)	Moisture content corresponding to second pressure head.	
.		
.		
.		
HK(ITEX,3*N1+5)	Moisture content corresponding to smallest pressure head.	
HK(ITEX,3*N1+6)	Always input a value of 99.	
Regardless of which functional relation is selected there must be NPROP+1 values on line B-7.		
Line B-7A is present only if TRANS = T.		
B-7A	HT(ITEX,1)	α_L, L.
	HT(ITEX,2)	α_T, L.
	HT(ITEX,3)	D_m, L^2T^{-1}.
	HT(ITEX,4)	λ, decay constant, T^{-1}.
	HT(ITEX,5)	ρ_b (can be set to 0 for no adsorption or ion exchange), ML^{-3}.
	HT(ITEX,6)	= 0 for no adsorption or ion exchange, = K_d for linear adsorption isotherm, = K_l for Langmuir isotherm, = K_f for Freundlich isotherm, = K_m for ion exchange.
	HT(ITEX,7)	= Q for Langmuir isotherm, = n for Freundlich isotherm (Note: n is a real, rather than an integer, variable), = $\hat{Q}$ for ion exchange, not used when adsorption is not simulated.
	HT(JTEX,8)	= C_0 for ion exchange, only used for ion exchanged.
B-8	IROW	If IROW = 0, textural classes are read for each row. This option is preferable if many rows differ from the others. IF IROW = 1, textural classes are read in by blocks of rows, each block consisting of all the rows in sequence consisting of uniform properties or uniform properties separated by a vertical interface.
Line set B-9 is present only if IROW = 0.		
B-9	JTEX	Indices (ITEX) for textural class for each node, read in row by row. There must be NLY*NXR entries.

Card	Variable	Description

Line set B-10 is present only if IROW = 1.

As many groups of B-10 variables as are needed to completely cover the grid are required. The final group of variables for this set must have IR = NXR and JBT = NLY.

B-10	IL	Left hand column for which texture class applies. Must equal 1 or [IR(from previous card)+1].
	IR	Right hand column for which texture class applies. Final IR for sequence of rows must equal NXR.
	JBT	Bottom row of all rows for which the column designations apply. JBT must not be increased from its initial or previous value until IR = NXR.
	JRD	Texture class within block.

Note: As an example, for a column of uniform material; IL = 1, IR = NXR, JBT = NLY, and JRD = texture class designation for the column material. One line will represent the set for this example.

B-11	IREAD	If IREAD = 0, all initial conditions in terms of pressure head or moisture content as determined by the value of PHRD are set equal to FACTOR. If IREAD = 1, all initial conditions are read from file IU in user-designated format and multiplied by FACTOR. If IREAD = 2 initial conditions are defined in terms of pressure head, and an equilibrium profile is specified above a free-water surface at a depth of DWTX until a pressure head of HMIN is reached. All pressure heads above this are set to HMIN.
	FACTOR	Multiplier or constant value, depending on value of IREAD, for initial conditions, L.

Line B-12 is present only if IREAD = 2,

B-12	DWTX	Depth to free-water surface above which an equilibrium profile is computed, L.
	HMIN	Minimum pressure head to limit height of equilibrium profile; must be less than zero, L.

Card	Variable	Description
Line B-13 is read only if IREAD = 1,		
B-13	IU	Unit number from which initial head values are to be read.
	IFMT	Format to be used in reading initial head values from unit IU. Must be enclosed in quotation marks, for example '(10X,E10.3)'.
B-14	BCIT	Logical variable = T if evaporation is to be simulated at any time during the simulation; otherwise = F.
	ETSIM	Logical variable = T if evapotranspiration (plant-root extraction) is to be simulated at any time during the simulation; otherwise = F.
Line B-15 is present only if BCIT = T or ETSIM = T.		
B-15	NPV	Number of ET periods to be simulated. NPV values for each variable required for the evaporation and/or evapotranspiration options must be entered on the following lines. If ET variables are to be held constant throughout the simulation code, NPV = 1.
	ETCYC	Length of each ET period, T.

Note: For example, if a yearly cycle of ET is desired and monthly values of PEV, PET, and the other required ET variables are available, then code NPV = 12 and ETCYC = 30 days. Then, 12 values must be entered for PEV, SRES, HA, PET, RTDPTH, RTBOT, RTTOP, and HROOT. Actual values, used in the program, for each variable are determined by linear interpolation based on time.

Line B-16 to B-18 are present only if BCIT = T.		
B-16	PEVAL	Potential evaporation rate (PEV) at beginning of each ET period. Number of entries must equal NPV, LT^{-1}.

To conform with the sign convention used in most existing equations for potential evaporation, all entries must be greater than or equal to 0. The program multiplies all nonzero entries by -1 so that the evaporative flux is treated as a sink rather than a source.

Card	Variable	Description
B-17	RDC(1,J)	Surface resistance to evaporation (SRES) at beginning of ET period, L^{-1}. For a uniform soil, SRES is equal to the reciprocal of the distance from the top active node to land surface, or 2./DELZ(2). If a surface crust is present, SRES may be decreased to account for the added resistance to water movement through the crust. Number of entries must equal NPV.
B-18	RDC(2,J)	Pressure potential of the atmosphere (HA) at beginning of ET period; may be estimated using equation 6 of Lappala and others (1987), L. Number of entries must equal NPV.
Lines B-19 to B-23 are present only if ETSIM = T.		
B-19	PTVAL	Potential evapotranspiration rate (PET) at beginning of each ET period, LT^{-1}. Number of entries must equal NPV. As with PEV, all values must be greater than or equal to 0.
B-20	RDC(3,J)	Rooting depth at beginning of each ET period, L. Number of entries must equal NPV.
B-21	RDC(4,J)	Root activity at base of root zone at beginning of each ET period, L^{-2}. Number of entries must equal NPV.
B-22	RDC(5,J)	Root activity at top of root zone at beginning of each ET period, L^{-2}. Number of entries must equal NPV.

Note: Values for root activity generally are determined empirically, but typically range from 0 to 3.0 cm/cm3. As programmed, root activity varies linearly from land surface to the base of the root zone, and its distribution with depth at any time is represented by a trapezoid. In general, root activities will be greater at land surface than at the base of the root zone.

B-23	RDC(6,J)	Pressure head in roots (HROOT) at beginning of each ET period, L. Number of entries must equal NPV.
Lines B-24 and B-25 are present only if TRANS = T.		
B-24	IREAD	If IREAD = 0, all initial concentrations are set equal to FACTOR. If IREAD = 1, all initial concentrations are read from file IU in user designated format and multiplied by FACTOR.

Card	Variable	Description
B-24--Continued	FACTOR	Multiplier or constant value, depending on value of IREAD, for initial concentrations.
Line B-25 is present only if IREAD = 1.		
B-25	IU	Unit number from which initial concentrations are to be read.
	IFMT	Format to be used in reading initial head values from unit IU. Must be enclosed in quotation marks, for example '(10X, E10.3)'.
[Line group C read by subroutine VSTMER, NRECH sets of C lines are required]		
C-1	TPER	Length of this recharge period, T.
	DELT	Length of initial time step for this period, T.
C-2	TMLT	Multiplier for time step length.
	DLTMX	Maximum allowed length of time step, T.
	DLTMIN	Minimum allowed length of time step, T.
	TRED	Factor by which time-step length is reduced if convergence is not obtained in ITMAX iterations. Values usually should be in the range 0.1 to 0.5. If no reduction of time-step length is desired, input a value of 0.0.
C-3	DSMAX	Maximum allowed change in head per time step for this period, L.
	STERR	Steady-state head criterion; when the maximum change in head between successive time steps is less than STERR, the program assumes that steady state has been reached for this period and advances to next recharge period, L.
C-4	POND	Maximum allowed height of ponded water for constant flux nodes. See Lappala ans others (1987) for detailed discussion of POND, L.
C-5	PRNT	Logical variable = T if heads, concentration, moisture contents, and/or saturations are to be printed to file 6 after each time step; = F if they are to be written to file 6 only at observation times and ends of recharge periods.
C-6	BCIT	Logical variable = T if evaporation is to be simulated for this recharge period; otherwise = F.

Card	Variable	Description
C-6--Continued	ETSIM	Logical variable = T if evapotranspiration (plant-root extraction) is to be simulated for this recharge period; otherwise = F.
	SEEP	Logical variable = T if seepage faces are to be simulated for this recharge period; otherwise = F
C-7 to C-9 cards are present only if SEEP = T,		
C-7	NFCS	Number of possible seepage faces. Must be less than or equal to 4.
Line sets C-8 and C-9 must be reported NFCS times		
C-8	JJ	Number of nodes on the possible seepage face.
	JLAST	Number of the node which initially represents the highest node of the seep; value can range from 0 (bottom of the face) up to JJ (top of the face).
C-9	J,N	Row and column of each cell on possible seepage face, in order from the lowest to the highest elevation; JJ pairs of values are required.
C-10	IBC	Code for reading in boundary conditions by individual node (IBC=0) or by row or column (IBC=1). Only one code may be used for each recharge period, and all boundary conditions for period must be input in the sequence for that code.
Line set C-11 is read only if IBC = 0. One line should be present for each node for which new boundary conditions are specified.		
C-11	JJ	Row number of node.
	NN	Column number of node.
	NTX	Node type identifier for boundary conditions. = 0 for no specified boundary (needed for resetting some nodes after intial recharge period); = 1 for specified pressure head; = 2 for specified flux per unit horizontal surface area in units of LT-1; = 3 for possible seepage face; = 4 for specified total head; = 5 for evaporation; = 6 for specified volumetric flow in units of L^3T^{-1}.

Card	Variable	Description
C-11--Continued	PFDUM	Specified head for NTX = 1 or 4 or specified flux for NTX = 2 or 6. If codes 0, 3, or 5 are specified, the line should contain a dummy value for PFDUM or should be terminated after NTX by a blank and a slash.
	NTC	Node type identifier for transport boundary conditions = 0 for no specified boundary; = 1 for specified concentration, ML^{-3}; = 2 for specified mass flux, MT^{-1}. Present only if TRANS = T.
	CF	Specified concentration for NTC = 1 or NTX = 1,2,4, or 6; or specified flux for NTC = 2. Present only if TRANS = T.
C-12 is present only if IBC = 1. One card should be present for each row or column for which new boundary conditions are specified,		
C-12	JJT	Top node of row or column of nodes sharing same boundary condition.
	JJB	Bottom node of row or column of nodes having same boundary condition. Will equal JJT if a boundary row is being read.
	NNL	Left column in row or column of nodes having same boundary condition.
	NNR	Right column of row or column of nodes having same boundary condition. Will equal NNL if a boundary column is being read in.
	NTX	Same as line C-11.
	PFDUM	Same as line C-11.
	NTC	Same as line C-11.
	CF	Same as line C-11.
C-13	Designated end of recharge period. Must be included after line C-12 data for each recharge period. Two C-13 lines must be included after final recharge period. Line must always be entered as 999999 /.	

MODEL IDENTIFICATION

Model Name
IGWMC Key
Date of First Release
Current Version Number
Current Version Release Date

Authors
Institution of Model Development
Code Custodian (contact person, address)
IGWMC Check Date

COMPUTER AND SOFTWARE SPECIFICATION

Computer systems for which versions exist (supercomputer, minicomputer, workstations, mainframe, microcomputer)
System requirements (RAM for execution, mass storage for programs and I/O files; numerical/math coprocessor, compiler required for main frame, MS Windows, other resident software
Graphics requirements (graphic board/monitor type/mode, resident graphic drivers)
Optional capabilities (plotter, printer, mouse)
Program information (programming language/ level, number of program statements, size of source code, size of runtime/compiled version)

Simulation Input Preparation or Preprocessing (textual data entry/editing, graphic data entry/modification, automatic grid generation, data reformatting, error-checking, help screens)
Data postprocessing (textual screen display, data storage in ASCII file, data directly to printer, graphic screen display of spatial data, graphic screen display of temporal data, direct graphic plotting, data reformatting

IGWMC EVALUATION

Primary Development Objective (research, e.g. hypothesis/theory testing; general use, e.g. in field applications; demonstration/ education)
Documentation (model theory, user's instructions, input preparation, model set-up, model options, example problems, demonstration of input/output illustrative of model options, program structure, program design/development, code listing, verification, validation)

Availability
- Terms (public domain, restricted public domain, proprietary, purchase, license)
- Form (source code only, compiled code only, source and compiled code, paper listing of source code

Code Use: few (<10); moderate (10-25); many(>25)
Verification/validation (verific. with analyt. solutions, verific. with synthetic datasets, testing with field datasets, testing with laboratory datasets, code inter-comparison)
Performance testing (stability, efficiency)
Peer (independent) review (concepts, theory, coding, accuracy, documentation, usability, efficiency)

Support
- Can be used without support
- Level of available support (full, limited, none, support agreement available)

GENERAL MODEL CAPABILITIES

Units (metric, S.I., U.S.)

Parameter discretization (lumped, water/mass balance model, response function model, distributed, stochastic)

Coupling (equations coupled, model modules coupled, internal software linkage, external I/O linkage)

Spatial orientation

saturated flow

- 1D
  - -horizontal
  - -vertical
- 2D
  - -horizontal (areal)
  - -vertical (crossectional/profile)
  - -axi-symmetric
- 3D
  - -fully-3D (definition in x,y,z)
  - -quasi-3D (layered; Dupuit approximation)
  - -cylindrical or radial

unsaturated flow

- 1D
  - -horizontal
  - -vertical
- 2D
  - -horizontal
  - -vertical
  - -axi-symmetric
- 3D
  - -fully-3D
  - -cylindrical or radial

Grid Design

Grid discretization applicable

- -constant cell size
- -variable grid size
- -movable grid (relocation of nodes during run)
- -automatic grid generation
- -maximum # of nodes

Possible cell shapes

- 1D
  - -linear
  - -curvilinear
- 2D
  - -triangular
  - -curved triangular
  - -square
  - -rectangular
  - -quadrilateral
  - -curved quadrilateral
  - -polygon
- 3D
  - -cubic
  - -hexahedral
  - -tetrahedral
  - -cylindrical
  - -spherical

REMARKS

REFERENCES

USERS

FLOW SYSTEM CHARACTERIZATION

Saturated zone

Hydrogeologic zoning (single aquifer, single aquifer/aquitard system, multiple aquifer/aquitard systems)

Aquifer type(s) present (confined, semi-confined or leaky confined, unconfined or phreatic)

Hydrogeologic medium (porous media, fractured media, discrete fractures, equivalent fracture approach, equivalent porous media approach, stochastic approach, dual porosity system or flow in fractures and porous blocks)

Flow characteristics (laminar flow Darcian flow, laminar non-Darcian flow, turbulent flow, steady-state, transient)

Flow parameter representation (homogeneous or heterogeneous, isotropic or anisotropic)

Well representation (partial penetration, filter dimensions, wellbore storage, skin effects)

Changing aquifer conditions in space (variable thickness, confined to unconfined or reverse, pinching aquifer, pinching aquitard)

Changing aquifer conditions in time (desaturation, confined/unconfined, resaturation of dry cells, parameter values)

Processes (areal recharge from surface, induced recharge from stream, aquitard storage, delayed yield from storage, freezing/thawing, vaporization/condensation, evaporation, evapotranspiration

Unsaturated Zone

Medium (porous media, layered porous media, aerially homogeneous or single soil type, aerially heterogeneous or multi soil types, macropores present, fractured media, dual porosity system, perched water table, dipping soil layers)

Flow characteristics (laminar Darcian flow, laminar non-Darcian flow, turbulent flow, steady-state, transient)

Processes:
- -infiltration(fixed head, fixed flux, ponding, infiltration function)
- -evaporation
- -evapotranspiration
- -plant uptake of water
- -capillary rise
- -hysteresis
- -interflow
- -swelling/shrinking soil matrix

Parameter definition (K_{sat}, suction vs. saturation, porosity, residual saturation, hydraulic conductivity vs. saturation, number of soil materials possible)

Soil moisture saturation - matric potential relationship (Brutsaert 1966, van Genuchten 1980, Haverkamp et al. 1977, tabular)

Soil hydraulic conductivity-saturation/hydraulic potential relationship (Wind 1955, Brooks and Corey 1966, van Genuchten 1980, Gardner 1958, Haverkamp et al. 1977, Averjanov 1950, Rijtema 1965, tabular)

Parameter representation (homogeneous, heterogeneous, isotropic, anisotropic)

Intercell conductance representation or K_r determination (arithmetic, harmonic, geometric)

FLUID CONDITIONS

Single fluid flow (water, vapor/gas/air, or nonaqueous-phase liquids)

Fluid properties (compressible fluid, spatially variable fluid density, temporally variable fluid density, density-temperature relationship, density-concentration relationship, variable viscosity)

Flow of multiple fluids (water and air/vapor, water and steam, salt-water and fresh-water with a sharp interface and either stagnant salt-water or moving salt-water and moving fresh-water, water and NAPL with about equal densities, water and DNAPL, water and LNAPL, liquid NAPL and gaseous NAPL)

BOUNDARY AND INITIAL CONDITIONS FOR FLOW

First type - Dirichlet:

- -head/pressure (constant in time, varying in time, cyclic functions)
- -prescribed moisture content (either constant in time or time-varying)

Second type - Neumann (either constant in time or time-varying):

- injection/production wells
- areal recharge in the saturated zone
- areal infiltration in the unsaturated zone
- no-flow
- cross-boundary flow

Third type - Cauchy:

- head-dependent flux (either constant in time or time-varying)
- -free surface (either constant in time or time-varying)
- -seepage face (either constant in time or time-varying)
- -springs
- -induced infiltration (from surface water)
- -ponding

Initial Conditions (saturation, moisture content, suction, total hydraulic head, hydraulic potential)

SOLUTION METHODS - FLOW MODELS

General Method:

Water balance approach

Analytical (single solution, superposition, method of images, analytical element method)

Semi-analytical (continuous in time and discrete in space, continuous in space and discrete in time, approximate analytical solution)

Numerical/spatial approximation (block-centered finite difference, node-centered finite difference, integrated finite difference, boundary element method, particle tracking, pathline integration, Galerkin finite element method, point collocation method, subdomain collocation method)

Numerical/time-stepping scheme (fully implicit, fully explicit, Crank-Nicholson)

Matrix-solving technique/Iterative (SIP, Gauss-Seidel or PSOR, LSOR, BSOR, Iterative ADIP or IADI, Predictor-corrector)

Matrix-solving technique/Semi-iterative (conjugate-gradient)

Matrix-solving technique/Direct (Gauss elimination, Cholesky decomposition, Frontal method, Doolittle, Thomas algorithm, Point Jacobi

Iterative methods for nonlinear equations (Picard method, Newton-Raphson method, Chord slope method)

INVERSE/PARAMETER IDENTIFICATION FOR FLOW

Parameters to be identified (hydraulic conductivity, transmissivity, storativity/ storage coefficient, leakeance/leakage factor, areal recharge, cross-boundary fluxes, pumping rates, soil parameters/ coefficients)

User input (prior information on variable to be determined, constraints on variable to be determined, instability conditions, non-uniqueness criteria, regularity conditions, aquifer properties, soil properties)

Parameter identification method/Direct method i.e. model parameters treated as dependent variable (energy dissipitation method, algebraic approach, inductive method or direct integration of PDE, minimizing norm of error flow or flatness criterion, linear programming, quadratic programming, matrix inversion)

Parameter identification method/Indirect method i.e. iterative improvement of parameter estimates (quasi-linearization, linear programming, quadratic programming, steepest descent, conjugate gradient, non-linear regression or Gauss-Newton method, Newton-Raphson, influence coefficient, maximum likelihood, co-kriging, gradient search, decomposition and multi-level optimization, least-squares)

OUTPUT CHARACTERISTICS - FLOW MODELS

Echo of input (nodal coordinates, cell size, element connectivity, initial heads/ pressures/potentials initial moisture content/saturation, soil parameters/ function coefficients, aquifer parameters, boundary conditions, stresses such as recharge and pumping)

Form of output (binary file, ASCII file with text, x-y[-z]/f{x,y,z} file, t/f{t} file, direct screen display, direct hardcopy on printer, direct plot on pen-plotter, graphic file)

Type of output:

- -head/pressure/potential (tables, contours, time series graphs)
- -saturation/moisture content (tables, contours, time series graphs)
- -head differential/drawdown (tables, contours, time series graphs)
- -internal (cross-cell) fluxes (tables, vector plots, time series graphs)
- -infiltration fluxes (tables, vector plots, time series graphs)
- -evapo(transpi)ration fluxes (tables, vector plots, time series graphs)
- -cross boundary fluxes (tables, vector plots, time series graphs)
- -velocities (tables, vector plots, time series graphs)
- -stream function values (tables, contours)
- -streamlines/pathlines (graphics)
- -traveltimes (tables)
- -isochrones (graphics)
- -position of interface (tables, graphics)
- -location of seepage faces
- -water budget components (cell-by-cell or global)
- -calculated parameters

WATER QUALITY CONSTITUENTS

Any constituent(s) vs. specific constituents (total dissolved solids, heavy metals, other metals, nitrates and nitrogen compounds, phosphates and phosphorus compounds, sulfates and sulphur compounds, chlorides, aromatic organic compounds, oxygenated organic compounds, halogenated organic compounds, micro-organisms, radionuclides)

Single vs. multi-species transport (single constituent, two constituents, multiple constituents)

PROCESSES

Conservative transport (uniform or non-uniform steady-state or transient advection, dispersion, molecular diffusion, plant solute uptake)

Phase transfers (solid<->gas or vapor sorption; solid<->liquid or liquid sorption including equilibrium isotherms such as linear, Langmuir, Freundlich, or non-equilibrium isotherms; desorption i.e. hysteresis; liquid->gas or volatilization; liquid->solids or filtration)

Parameter representation:
-dispersivity (isotropic i.e. $a_T = a_L$, anisotropic, homogeneous i.e. constant in space, heterogeneous)
-diffusion coefficient (homogeneous, heterogeneous)
-retardation factor (homogeneous, heterogeneous)

Fate:
-Type of reactions (ion exchange, substitution/hydrolysis, dissolution/precipitation, reduction/oxidation, acid/base reactions, complexation, aerobic or anaerobic biodegradation)
-Form of reactions (zero order production/decay, first order production/decay, chemical production/decay, radioactive decay including single mother/daughter decay and chain decay, microbial production/decay with Monod functions for aerobic biodegradation or Michaelis-Menten function for anaerobic biodegradation)

Chemical processes embedded in transport equation or given by separate equation(s)

BOUNDARY CONDITIONS FOR SOLUTE TRANSPORT

First type - Dirichlet: concentration (constant in time, varying in time, at domain boundary, at injection wells if flow rate is given)

Second type - Neumann: prescribed solute flux (constant in time or time-varying, point sources e.g. injection wells, line sources e.g. infiltration ditches, areal sources e.g. feedlots and landfills, non-point or diffuse sources)

SOLUTION METHODS - SOLUTE TRANSPORT MODELS

Flow and solute transport equations are uncoupled or coupled (through concentration-dependent density or viscosity).

SOLUTION METHODS - SOLUTE TRANSPORT MODELS (continued)

General Method:

-Solute mass balance approach, analytical (single solution, superposition), semi-analytical (continuous in time and discrete in space, continuous in space and discrete in time, approximate analytical solution)

Numerical/time-stepping scheme (fully implicit, fully explicit, Crank-Nicholson)

Matrix-solving technique/Iterative (SIP, Gauss-Seidel or PSOR, LSOR, BSOR, Iterative ADIP or IADI, Predictor-corrector)

Matrix-solving technique/Semi-iterative (conjugate-gradient)

Numerical/spatial approximation (block-centered finite difference, node-centered finite difference, integrated finite difference, boundary element method, particle tracking, method of characteristics, random walk method, Galerkin finite element method, point collocation method, subdomain collocation method)

Matrix-solving technique/Direct (Gauss elimination, Cholesky decomposition, Frontal method, Doolittle, Thomas algorithm, Point Jacobi

Iterative methods for nonlinear equations (Picard method, Newton-Raphson method, Chord slope method)

INVERSE/PARAMETER IDENTIFICATION FOR SOLUTE TRANSPORT

Parameters to be identified (velocity, dispersivity, diffusion coefficient, retardation factor, source strength, initial conditions in terms of concentrations)

Parameter identification method/Direct method i.e. model parameters treated as dependent variable (energy dissipitation method, algebraic approach, inductive method or direct integration of PDE, minimizing norm of error flow or flatness criterion, linear programming, quadratic programming, matrix inversion)

User input (prior information, constraints, instability conditions, non-uniqueness criteria, regularity conditions)

Parameter identification method/Indirect method i.e. iterative improvement of parameter estimates (linear or quadratic programming, steepest descent, conjugate gradient, non-linear regression, Newton-Raphson, influence coefficient, maximum likelihood, co-kriging, gradient search, least-squares)

OUTPUT CHARACTERISTICS - SOLUTE TRANSPORT MODELS

Echo of input (initial concentrations, parameter values, boundary conditions, stresses i.e. source fluxes)

Type of output:

-concentration values (tables, contours, time series graphs)

-concentration in pumping wells (time series tables and graphs)

-calculated parameters

Form of output (binary file, ASCII file with text, x-y[-z]/f{x,y,z} file, t/f{t} file, direct screen display, direct hardcopy on printer, direct plot on pen-plotter, graphic file)

-internal and cross-boundary solute fluxes (tables, vector plots, time series graphs)

-velocities (from given heads)

-mass balance components (cell-by-cell or global)

PROCESSES

Transport processes (uniform or non-uniform steady-state or transient convection, conduction through rock-matrix, conduction through liquid, thermal dispersion, thermal diffusion between rock matrix and liquid, radiation)

Phase change (evaporation and condensation, water and vapors, water and steam, freezing and thawing, heat exchange between phases)

Internal heat generation (internal heat source)

Parameter representation (parameters not mentioned are considered homogeneous in space):

-thermal conductivity of rock matrix (homogeneous, heterogeneous)

-thermal dispersion coefficient (isotropic i.e. $a_T = a_L$, anisotropic, homogeneous i.e. constant in space, heterogeneous)

BOUNDARY CONDITIONS FOR HEAT TRANSPORT

First type - Dirichlet: temperature (constant in time or time-varying source at domain boundary or at injection wells)

Third type - Cauchy: given geothermal gradient

Second type - Neumann: heat flux (constant in time or time-varying release at point sources, line sources, areal sources, or non-point diffuse sources)

SOLUTION METHODS - HEAT TRANSPORT MODELS

Flow and heat transport equations are uncoupled or coupled (through temperature-dependent density or viscosity).

General Method: Heat or energy balance approach, analytical (single solution, superposition), semi-analytical (continuous in time and discrete in space, continuous in space and discrete in time, approximate analytical solution)

Numerical/time-stepping scheme (fully implicit, fully explicit, Crank-Nicholson)

Matrix-solving technique/Iterative (SIP, Gauss-Seidel or PSOR, LSOR, BSOR, Iterative ADIP or IADI, Predictor-corrector)

Matrix-solving technique/Semi-iterative (conjugate-gradient)

Numerical/spatial approximation (block-centered finite difference, node-centered finite difference, integrated finite difference, boundary element method, particle tracking, method of characteristics, random walk method, Galerkin finite element method, point collocation method, subdomain collocation method)

Matrix-solving technique/Direct (Gauss elimination, Cholesky decomposition, Frontal method, Doolittle, Thomas algorithm, Point Jacobi

Iterative methods for nonlinear equations (Picard method, Newton-Raphson method, Chord slope method)

OUTPUT CHARACTERISTICS - HEAT TRANSPORT MODELS

Echo of input (initial temperatures, parameter values, boundary conditions, stresses i.e. source fluxes)

Form of output (binary file, ASCII file with text, x-y[-z]/f{x,y,z} file, t/f{t} file, direct screen display, direct hardcopy on printer, direct plot on pen-plotter, graphic file)

OUTPUT CHARACTERISTICS - HEAT TRANSPORT MODELS (continued)

Type of output:

- -temperature values (tables, contours, time series graphs)
- -temperature in pumping wells (time series tables and graphs)
- -calculated parameters
- -frost front location (tables, graphs)
- -internal and cross-boundary heat fluxes (tables, vector plots, time series graphs)
- -velocities (from given heads)
- -heat/energy balance components (cell-by-cell or global)

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