Global Journal of Engineering Science and Research Management

MODELLING FLOW AND TRANSPORT IN UNSATURATED ZONE

C. P. KUMAR*
*Scientist 'G', National Institute of Hydrology, Roorkee – 247667, Uttarakhand, India..

KEYWORDS: Groundwater, Richards Equation, Numerical Modelling, Hydraulic Conductivity, Moisture Content.

ABSTRACT
Unsaturated zone transport models are indispensable tools for analyzing complex environmental pollution problems, and for developing practical management strategies. A quantitative study of water flow and contaminant transport in the unsaturated (vadose) zone is necessary for improvement and protection of the quality of groundwater supplies. This is the region bounded above by the land surface and below by the groundwater table. It is the region through which water derived from precipitation and irrigation infiltrates and transports contaminants to reach the groundwater. This article presents an overview of the modelling process for water flow and contaminant transport in the unsaturated zone, input data requirements and related software packages.

INTRODUCTION
The unsaturated zone is the region through which water, together with pollutant carried by the water, must pass to reach the groundwater. Therefore various processes occurring within the unsaturated zone play a major role in determining both the quality and quantity of water recharging into the groundwater. A quantitative study of water flow and contaminant transport in the unsaturated zone is a key factor in the improvement and protection of the quality of groundwater supplies.

Numerous simulation models for water flow and solute transport in the unsaturated zone are now being used increasingly for numerous applications in both research and management. Modelling techniques vary from straightforward analytical or semi-analytical methods to sophisticated numerical codes. Although analytical and semi-analytical methods remain widely used for certain applications, the growing power of personal computers along with the progression of more precise and numerically stable solution techniques have inspired significantly broader usage of numerical codes in recent years. The extensive utilization of numerical models is additionally greatly improved by their availability in both the commercial and public domains, and by the advancement of innovative graphics-based interfaces which significantly simplify their usage.

MATHEMATICAL EQUATIONS OF WATER AND TRANSPORT IN UNSATURATED SOILS
Analytical, semi-analytical, and numerical models are usually based on the following three governing equations for water flow, solute transport, and heat movement, respectively:

$$\frac{\partial \theta(h)}{\partial t} = \frac{\partial}{\partial z}\left[K(h)\left(\frac{\partial h}{\partial z} + 1\right)\right] - S \quad \text{... (1)}$$

$$\frac{\partial \theta R c}{\partial t} = \frac{\partial}{\partial z}\left[\theta D\left(\frac{\partial c}{\partial z}\right) - qc\right] - \emptyset \quad \text{... (2)}$$

$$\frac{\partial C(\theta) T}{\partial t} = \frac{\partial}{\partial z}\left[\lambda(\theta)\left(\frac{\partial T}{\partial z}\right) - C_w q T\right] \quad \text{... (3)}$$

Suitable simplifications (mostly for analytical approaches) or extensions thereof (e.g. for two- and three-dimensional systems) are also employed. In equation (1), frequently known as the Richards equation, h is the pressure head, z is the vertical coordinate positive upwards, θ is the water content, t is time, *S* is a sink term representing root water uptake or some other sources or sinks, and the hydraulic conductivity function (unsaturated) *K(h)* is, often given as the product of the relative hydraulic conductivity, K_r, and the saturated hydraulic conductivity, K_s. In equation (2), called the *convection-dispersion equation* (CDE), *c* is the solution concentration, D is the dispersion coefficient accounting for hydrodynamic dispersion and molecular diffusion, the retardation factor (R) that accounts for adsorption, the volumetric fluid flux density (*q*), and Φ is a sink/source term that accounts for various zero- and first-order or other reactions. In equation (3), *T* is temperature, λ is the apparent thermal conductivity, and *C* and C_w are the volumetric heat capacities of the soil and the liquid phase, respectively.

ISSN 2349-4506
Impact Factor: 2.265
Global Journal of Engineering Science and Research Management

Solutions of the Richards equation (1) require knowledge of the unsaturated soil hydraulic functions, that is, the soil water retention curve, *θ(h)*, describing the relationship between the water content *θ* and the pressure head *h*, and the hydraulic conductivity function (unsaturated), *K(h)*, defining the hydraulic conductivity *K* as a function of *h* or *θ*. Under certain conditions (i.e. for linear sorption, a concentration-independent sink term *Φ*, and a steady flow field), equations (2) and (3) are linear equations. But equation (1) is often very nonlinear due to the nonlinearity of the soil hydraulic properties. Consequently, numerous analytical solutions were derived previously for equations (2) and (3) and these analytical solutions are still popular for evaluating solute and heat transport under steady-state conditions. Although a large number of analytical solutions of (1) exist, they can generally be applied only to drastically simplified problems. Most of the applications of water flow in the vadose zone demand a numerical solution of the Richards equation.

REQUIRED INPUT DATA

Simulation of water dynamics in the unsaturated zones needs input data regarding the model parameters, the geometry of the system, the boundary conditions and when simulating transient flow, initial conditions also. With geometry parameters, the dimensions of the problem domain are defined. With the physical parameters, the physical properties of the system under consideration are described. In relation to the unsaturated zone, it concerns h(θ) (soil water characteristic), and K(θ) (hydraulic conductivity).

For an appropriate explanation of the unsaturated flow, a proper description of the two hydraulic functions, h(θ) and K(θ), is important. K(θ), the hydraulic conductivity, decreases significantly when the moisture content (θ) decreases from saturation. The experimental approach to measure K(θ) at different moisture contents is fairly complicated and not too trustworthy. Alternate methods were therefore developed to determine the K(θ) function from more conveniently measurable characterizing properties of the soil. In many studies, the hydraulic conductivity of the unsaturated soil is defined as product of a non-linear function of the effective water saturation, together with hydraulic conductivity at saturation. The relationship is shown by

$$K(\theta) = K_s \left(\frac{\theta - \theta_r}{\theta_s - \theta_r} \right)^n \qquad \dots (4)$$

where,

K_s = hydraulic conductivity at saturation;
θ_s = saturated water content; and
θ_r = residual water content.

The value of n is found to be 3.5 for coarse textured soils. n will vary with soil type. In literature, established empirical correlation between n and soil characteristic is available. The relationship between the soil water pressure head h(θ) and moisture content θ, termed as the soil moisture characteristic or water retention curve, is normally determined by the textural and the structural composition of the soil. Also, the organic matter content may have an influence on the relationship. A characteristic feature of the water retention curve is that suction head (-h) decreases fairly rapidly with increasing moisture content. Hysteresis effects might emerge, and rather than being a single-valued relationship, the h-θ relation includes a group of curves. The actual curve will have to be determined from the history of wetting and drying.

When root water uptake is also modelled, the parameters describing the relation between root water uptake together with soil water status has to be supplied, along with crop specifications. If a functional flux-head relationship is employed as lower boundary condition, the parameters describing the interaction between surface water and groundwater and, if required, the vertical resistance of low permeable layers must be provided.

The number and kind of parameters necessary for modelling flow as well as transport processes in soils are dependent on the kind of model selected. These parameters can be categorized as 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 seven sets (Jury and Valentine, 1986) – static soil properties, water transport and retention functions, time-dependent parameters, basic chemical properties, contaminant source characteristics, soil adsorption parameters, and tortuosity functions. Table 1 lists many of the relevant material model parameters.

Table 1: Selected material parameters for flow and transport modelling

<table>
<tr><th colspan="3">Model Parameters</th></tr>
<tr><td>Static Soil Properties

Porosity
Bulk Density
Particle Size
Specific Surface Area
Organic Carbon Content
Cation Exchange Capacity
pH
Soil Temperature</td><td>Flow and Transport Variables and Properties

Saturated Hydraulic Conductivity
Saturated Water Content
Moisture Retention Function
Hydraulic Conductivity Function
Dispersion Coefficient</td><td>Basic Chemical Properties

Molecular Weight
Vapour Pressure
Water Solubility
Henry's Constant
Vapour Diffusion Coeff. in air
Liquid Diffusion Coeff. in water
Half-life or decay Rate
Hydrolysis Rate (s)</td></tr>
<tr><td rowspan="3">Time Dependent Parameters

Water Content
Water Flux
Infiltration Rate
Evaporation Rate
Solute Concentration
Solute Flux
Solute velocity
Air Entry Pressure Head
Volatization Flux</td><td colspan="2">Contaminant Source Characteristics

Solute Concentration of Source
Solute Flux of Source
Source Decay Rate</td></tr>
<tr><td colspan="2">Soil Adsorption Parameters

Distribution Coefficient
Isotherm Parameters
Organic Carbon Partition Coefficient</td></tr>
<tr><td colspan="2">Tortuosity Functions

Vapour Diffusion Tortuosity
Liquid Diffusion Tortuosity</td></tr>
</table>

MODELLING OF UNSATURATED FLOW

Analytical solutions, if available, offer a greater understanding of the physics behind the transport phenomena and are computationally efficient and simple to use. However, analytical approaches are for the most part limited to situations of simple geometry domains, linear governing equations, and homogeneous systems. Along with efficient numerical methods and rapidly updated computer hardware, a large number of numerical models have been developed. However, the numerical technique can not replace the analytical approaches completely, since numerical methods themselves need verification against analytical solutions because of discretization errors and convergence and stability problems that may be especially troublesome for advection-dominated and nonlinear adsorption processes.

Analytical solutions to the Richards equation for unsaturated flow under various boundary and initial conditions are difficult to obtain because of the nonlinearity in soil hydraulic parameters. This difficulty is exaggerated in the case where the soil is heterogeneous. Usually, one has to depend on numerical methods for predicting moisture movement in unsaturated soils, even for soils that are homogeneous. However, numerical approaches often suffer from convergence and mass balance problems.

Analytical solutions are only applicable to highly simplified systems and are not well suited for situations normally encountered in the field. Originally, finite difference techniques were primarily formulated to predict unsaturated flow solely; however finite element solution methods also were introduced later on. The nonlinearity of Richards equation is usually solved using an iterative procedure such as Newton or Picard methods. Perhaps the most important advantage of finite element techniques over standard finite difference methods is the ability to describe irregular system boundaries in simulations more accurately, as well as easily including non-homogeneous medium properties. For one-dimensional simulations, finite difference methods are just as good as finite element schemes. However, several authors suggest that finite element methods lead to more stable and accurate solutions, thus permitting larger time steps and/or coarser grid systems, and hence leading to

 ISSN 2349-4506
Impact Factor: 2.265
Global Journal of Engineering Science and Research Management

computationally more efficient numerical schemes.

To numerically solve coupled systems of equations, the solution process requires some manipulation at each time step so that the dependence of one equation on the solution of the other is dealt with accurately. One way to overcome this is to use a fully implicit approach to solve the equations simultaneously. Any nonlinearity of the generated system can be handled by Newton's method. The implicit nature of this scheme allows for larger time steps in the simulation to find stable solutions as compared to the time steps for explicit schemes. An alternative to fully implicit scheme is to apply the mixed implicit-explicit approach. Yet somehow, the explicit portion of the scheme implies that this algorithm is now dependent upon a stability constraint which significantly limits the size of the time step and opens up numerical artifacts.

For heterogeneous soils that contain macro-pores, a different modelling approach is needed, as the presence of macro-pores in these soils may form a separate network for water flow. The common approach is to introduce two-region flow domain, one for macro-pores and the other for the soil matrix. In each flow domain, hydraulic conductivity is given independently. One more strategy would be to think of the heterogeneous soil as a group of stream tubes. It is assumed that there is no exchange of water between these tubes and that within each tube, the hydraulic conductivity is defined, but varies between tubes.

MODELLING OF SOLUTE TRANSPORT

Movement of dissolved solutes in soils is often defined by the advection-dispersion equation. Analytical solutions have been derived for various boundary and initial conditions. Although these solutions are obtained for limited specified conditions, they have numerous applications like the verification of computer codes, prediction of solute movement for large times or distances where the use of numerical models become impractical, and the determination of transport parameters from soil column tests. The majority of analytical solutions pertain to semi-infinite and infinite media. Solutions are obtained by a variety of mathematical techniques including Green's functions, separation of variables, characteristics method, Laplace transforms and Fourier transforms.

Prediction of solute migration under field situations requires the concurrent solution of the solute transport and unsaturated flow equations. First approximations involve or assume steady flow and constant water contents. Because of the natural complexity of unsaturated flow, strategies for predicting solute transport have depended mostly on the finite difference or finite element approximations of the governing equations. Given that the equations for advection-diffusion transport usually do not have closed form analytical solutions, it is crucial that the numerical approximations be correct. When diffusion dominates the physical process, regular finite difference and finite element methods function effectively in solving these equations. But if advection is the dominant process, these equations could display numerous numerical problems. In fact, any standard finite difference or finite element method will produce a solution, which exhibits non-physical oscillations.

One of the distinctive features of the porous media on the field scale is the spatial heterogeneity of transport properties. These features have a distinct effect on the spatial distribution of contaminant concentration, as has been observed in field experiments and demonstrated by simulation of contaminant transport in unsaturated, heterogeneous soil. Description of the mixing process due to spatial variability of the unsaturated hydraulic conductivity has been advanced with the development of numerical solutions, which assume spatially variable soil properties; stochastic models; and stochastic stream tube models, which decompose the field into a set of independent vertical soil columns.

UNSATURATED ZONE MODELLING SOFTWARE

Most of the early models developed for studying processes in the near-surface environment focused mainly on variably saturated water flow. They were used primarily in agricultural research for the purpose of optimizing moisture conditions to increase crop production. This focus has increasingly shifted to environmental research, with the primary concern now being the subsurface fate and transport of various agricultural and other contaminants. While the earlier models solved the governing equations (1) through (3) for relatively simplified system-independent boundary conditions (i.e. specific pressure heads or fluxes, together with free water drainage), models developed recently could handle even more intricate system-dependent boundary conditions analyzing energy balances and surface flow and accounting for the concurrent movement of heat, vapour and water. There are also composite models which simulate the processes both in unsaturated and saturated zones and other components of the hydrological cycle. Few of the widely used unsaturated flow and composite models have been listed in Table 2.

Table 2: Numerical models for simulating unsaturated flow and solute transport

S.No.	Modelling Software	Salient Features
Unsaturated Flow Models		
1.	HYDRUS-1D	Public domain modelling environment for analysis of water flow and solute transport; includes the one-dimensional finite element model HYDRUS for simulating the movement of water, heat, and multiple solutes in variably saturated media; supported by an interactive graphics-based interface for data-preprocessing, discretization of the soil profile, and graphic presentation of the results.
2.	HYDRUS 2D/3D	Software package for simulating water, heat, and solute movement in two- and three-dimensional variably saturated media; consists of a computational computer program and an interactive graphics-based user interface.
3.	R-UNSAT	USGS computer model for the simulation of reactive, multispecies transport in a heterogeneous, variably-saturated porous media; designed for simulating transport of volatile organic compounds in the unsaturated zone from point and nonpoint sources; can also be applied to other unsaturated-zone transport problems involving gas diffusion, such as radon migration and the deposition of compounds from the atmosphere to shallow groundwater.
4.	SWIM	A mechanistically-based model designed to address soil water and solute balance issues in unsaturated zone.
5.	UNSAT SUITE	Handle one-dimensional groundwater flow and contaminant transport in the unsaturated zone; simulates the downward vertical flow of groundwater and migration of dissolved contaminants in the groundwater through a thin column of soil.
6.	VS2DI	USGS graphical software package for simulating fluid flow and solute or energy transport in variably saturated porous media.
Composite Models		
7.	FEFLOW	Commercial software based on the finite element method for simulation of saturated and unsaturated flow, transport of mass (multiple solutes) and heat, with integrated GUI.
8.	HydroGeoSphere	Commercial three-dimensional control-volume finite element simulator designed to simulate the entire terrestrial portion of the hydrologic cycle; uses a globally-implicit approach to simultaneously solve the 2D diffusive-wave equation and the 3D form of Richards' equation.
9.	MIKE SHE	Commercial software for integrated catchment modelling, with integrated GUI; uses the finite difference method for saturated groundwater flow, several representations of unsaturated flow, including the 1D Richards equation, MIKE 11 for flow in river and stream networks and the 2D diffusive-wave approach for overland flow.
10.	MODFLOW-SURFACT	Commercial software for simulation of saturated and unsaturated flow and solute transport: developed to overcome specific limitations in open source versions of MODFLOW and MT3D: also available in an extended form called MODHMS, which includes 2D diffusive wave simulation of overland flow and 1D simulation of flow in river and stream networks.
11.	SUTRA	Open source USGS software based on the finite element method for simulation of saturated and unsaturated flow, transport of mass and heat. It has been designed for density-coupled flow and transport.

CONCLUDING REMARKS

Predicting water movement and contaminant transport on a field-scale according to the existing monitoring and modelling methods is a challenging task. The accuracy of the obtained predictions depend to a large extent upon the accuracy of available model input parameters and upon the proper conceptualization of soil heterogeneity and

ISSN 2349-4506
Impact Factor: 2.265

Global Journal of Engineering Science and Research Management

other system complexities, such as the possible presence of non-equilibrium flow and transport, including preferential flow. Processes are often described and their parameters measured on a much smaller scale than those for which the model predictions are being sought. Consequently, many model parameters often need to be calibrated so that they reflect the bulk behaviour of the heterogeneous system, in which case they can be used for larger scale predictions.

Models can help guide field observations by identifying which parameters and processes control system behaviour. Even so, there are large uncertainties in prediction mostly because of our inability to demonstrate detailed spatial distributions of soil hydraulic properties on the field-scale. Due to the high costs of data acquisition, only few field measurements are usually available for the characterization of flow and contaminant transport, although the spatial distribution of a contaminant plume could be very irregular. New measuring techniques that provide model parameters on the scale at which predictions are made are badly needed for successful applications of unsaturated flow and transport models in a predictive mode at the larger scale. Also, more research associated with the flow of water along with contaminant transport in the unsaturated zone of aquifers containing fractures and karstic conduits is needed for future investigations.

One may expect that unsaturated zone flow and transport models will be used increasingly for integrating fundamental knowledge about the vadose zone to yield tools for developing cost-effective, yet technically sound strategies for resource management and pollution remediation and prevention.

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