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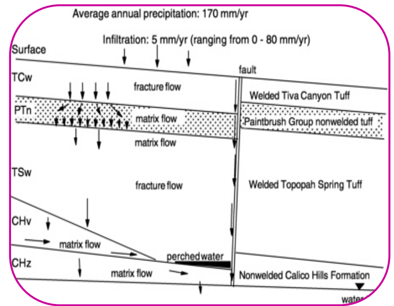
MODELLING WATER FLOW IN UNSATURATED ZONE



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ABSTRACT

The water movements in the unsaturated zone, together with the water holding capacity of this zone, are very important for the water demand of the vegetation, as well as for the recharge of the groundwater storage. A fair description of the flow in the unsaturated zone is crucial for predictions of the movement of pollutants into groundwater aquifers. This article presents an overview of the modelling process for water flow in the unsaturated zone, input data requirements, boundary conditions and related software packages.

KEYWORDS: *hydraulic conductivity, moisture content, Richards equation, evapotranspiration, groundwater recharge, HYDRUS.*

1.0 INTRODUCTION:-

Subsurface formations containing water may be divided vertically into several horizontal zones according to how large a portion of the pore space is occupied by water. Essentially, we have a zone of saturation in which all the pores are completely filled with water, and an overlaying zone of aeration in which the pores contain both gases (mainly air and water vapour) and water. The latter zone is called the unsaturated zone. Sometimes the term soil water is used for the water in this zone.

Various processes occurring within the unsaturated zone play a major role in determining the quality and quantity of water recharge to the groundwater. A quantitative analysis 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.

For analytical studies on soil moisture regime, critical review and accurate assessment of the different controlling factors is necessary. The controlling factors of soil moisture may be classified under two main groups viz. climatic factors and soil factors. Climatic factors include precipitation data containing rainfall intensity, storm duration, inter-storm period, temperature of soil surface, relative humidity, radiation, evaporation, and evapotranspiration. The soil factors include soil matric potential and water content relationship, hydraulic conductivity and water content relationship of the soil, saturated hydraulic conductivity, and effective medium porosity. Besides these factors, the information about depth to water table is also required.

Most of the processes involving soil-water interactions in the field, and particularly the flow of water in the rooting zone of most crop plants, occur while the soil is in an unsaturated condition. Unsaturated flow processes are in general complicated and difficult to describe quantitatively, since they often entail changes in the state and content of soil water during flow. Such changes involve complex relations among the variable soil wetness, suction, and conductivity, whose inter-relations may be further complicated by hysteresis.

The formulation and solution of unsaturated flow problems very often require the use of indirect methods of analysis, based on approximations or numerical techniques. For this reason, the development of rigorous theoretical and experimental methods for treating these problems was rather late in coming. In recent decades, however, unsaturated flow has become one of the most important and active topics of research and this research has resulted in significant theoretical and practical advances.

2.0 GOVERNING EQUATIONS OF WATER AND TRANSPORT IN UNSATURATED SOILS:-

Analytical, semi-analytical, and numerical models are used for unsaturated zone modelling. These 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), often referred to as the Richards equation, z is the vertical coordinate positive upwards, t is time, h is the pressure head, ϑ is the water content, S is a sink term representing root water uptake or some other sources or sinks, and $K(h)$ is the unsaturated hydraulic conductivity function, often given as the product of the relative hydraulic conductivity, K_r, and the saturated hydraulic conductivity, K_s. In equation (2), known as the *convection-dispersion equation* (CDE), c is the solution concentration, R is the retardation factor that accounts for adsorption, D is the dispersion coefficient accounting for both molecular diffusion and hydrodynamic dispersion, q is the volumetric fluid flux density, 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.

Solutions of the Richards equation (1) require knowledge of the unsaturated soil hydraulic functions, that is, the soil water retention curve, $\vartheta(h)$, describing the relationship between the water content ϑ and the pressure head h, and the unsaturated hydraulic conductivity function, $K(h)$, defining the hydraulic conductivity K as a function of h or ϑ. While 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; equation (1) is generally highly nonlinear because of the nonlinearity of the soil hydraulic properties. Consequently, many analytical solutions have been derived in the past for equations (2) and (3) and these analytical solutions are now widely used for analyzing 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. The majority of applications for water flow in the vadose zone require a numerical solution of the Richards equation.

3.0 INPUT DATA FOR UNSATURATED ZONE MODELLING:-

Simulation of water dynamics in the unsaturated zones requires input data concerning the model parameters, the geometry of the system, the boundary conditions and, when simulating transient flow, initial conditions. 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. With respect to the unsaturated zone, it concerns the soil water characteristic, $h(\theta)$ and the hydraulic conductivity, $K(\theta)$.

To model the retention, movement of water and chemicals in the unsaturated zone, it is necessary to know the relationships between soil water pressure, water content and hydraulic conductivity. It is often convenient to represent these functions by means of relatively simple parametric expressions. The problem of characterizing the soil hydraulic properties then reduces to estimating parameters of the appropriate constitutive model. The measurements of $\theta(h)$ from soil cores (obtained through pressure plate apparatus) can be fitted to the desired soil water retention model. Once the retention function is estimated, the hydraulic conductivity relation, $K(h)$, can be evaluated if the saturated hydraulic conductivity, K_s, is known. A number of models for water retention function and unsaturated hydraulic conductivity are well reported in literature, one of the most popular being van Genuchten model. For the van Genuchten (1980) model, the water retention function is given by

$$S_e = (\theta - \theta_r)/(\theta_s - \theta_r) = [\, 1 + (\alpha_v |h|)^n]^{-m} \qquad \text{for } h < 0$$
$$= 1 \qquad \text{for } h \geq 0 \qquad \dots (4)$$

and the hydraulic conductivity function is described by

$$K = K_s S_e^{1/2} [\, 1 - (1 - S_e^{1/m})^m]^2 \qquad \dots (5)$$

where, α_v and n are van Genuchten model parameters, $m = 1 - 1/n$, subscript s refers to saturation, i.e. the value of θ for which $h = 0$, and the subscript r to residual water content.

The number and type of parameters required for modelling flow and transport processes in soils depend on the type of model chosen. 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

Model Parameters		
Static Soil Properties	*Flow and Transport Variables and Properties*	*Basic Chemical Properties*
Porosity	Saturated Hydraulic Conductivity	Molecular Weight
Bulk Density	Saturated Water Content	Vapour Pressure
Particle Size	Moisture Retention Function	Water Solubility
Specific Surface Area	Hydraulic Conductivity Function	Henry's Constant
Organic Carbon Content	Dispersion Coefficient	Vapour Diffusion Coeff. in air
Cation Exchange Capacity		Liquid Diffusion Coeff. in water
pH		Half-life or decay Rate
Soil Temperature		Hydrolysis Rate (s)
Time Dependent Parameters	*Contaminant Source Characteristics*	
Water Content	Solute Concentration of Source	
Water Flux	Solute Flux of Source	
Infiltration Rate	Source Decay Rate	
Evaporation Rate	*Soil Adsorption Parameters*	
Solute Concentration		
Solute Flux	Distribution Coefficient	
Solute velocity	Isotherm Parameters	
Air Entry Pressure Head	Organic Carbon Partition Coefficient	

Volatization Flux	*Tortuosity Functions* Vapour Diffusion Tortuosity Liquid Diffusion Tortuosity

4.0 MODELLING OF UNSATURATED FLOW:-

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 as well as governing equation. This difficulty is exaggerated in the case where soil is heterogeneous. Generally, one has to rely on numerical approaches for predicting moisture movement in unsaturated soils, even for homogeneous soils. However, numerical approaches often suffer from convergence and mass balance problems. 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.

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 the fully implicit scheme is to use the mixed implicit-explicit scheme. However, the explicit part of the scheme means that this algorithm is now subject to a stability constraint which severely restricts the size of the time step and introduces numerical artefacts.

4.1 Initial and Boundary Conditions

Initial conditions must be defined when transient soil water flow is modeled. Usually values of matric head or soil water content at each nodal point within the soil profile are required. When these data are not available, water contents at field capacity or those in equilibrium with the groundwater table might be considered as the initial ones.

While the potential evapotranspiration rate from a soil depends on crop and atmospheric conditions, the actual flux through the soil surface and the plants is limited by the ability of the soil matrix to transport water. Similarly, if the potential rate of infiltration exceeds the infiltration capacity of the soil, part of the water runs off, since the actual flux through the top layer is limited by moisture conditions in the soil. Consequently, the exact boundary conditions at the soil surface cannot be estimated a priori and solutions must be found by maximizing the absolute flux. The minimum allowed pressure head at the soil surface, h^{lim} (time dependent) can be determined from equilibrium conditions between soil water and atmospheric vapour. The possible effect of ponding has been neglected so far. In case of ponding, usually the height of the ponded water as a function of time is given. However, when the soil surface is at saturation then the problem is to define the depth in the soil profile where the transition from saturation to partial saturation occurs.

In most of the dynamic transient models, the surface nodal point is treated during the first iteration as a prescribed flux boundary and matric head h is computed. If $h^{lim} \leq h \leq 0$, the upper boundary condition remains a flux boundary during the whole iteration. If not, the surface nodal point is treated as a prescribed pressure head in the following iteration. Then in case of infiltration, h = 0 and in case of evaporation $h = h^{lim}$. The actual flux is then calculated explicitly and is subject to the condition that actual upward flux through the soil-air interface is less than or equal to potential evapotranspiration (time dependent).

At the lower boundary, one can define three different types of conditions: (a) Dirichlet condition, the pressure head is specified; (b) Neumann condition, the flux is specified; and (c) Cauchy condition, the flux is a function of a dependent variable. The phreatic surface (place, where matric head is atmospheric) is usually taken as lower boundary of the unsaturated zone in the case where recorded water table fluctuations are known a priori. Then the flux through the bottom of the system can be calculated. In regions with a very deep groundwater table, a Neumann type of boundary condition is used.

4.2 Evapotranspiration (water extraction by roots)

In the field, steady-state conditions hardly exist. The living root system is dynamic (dying roots are constantly replaced by new ones), geometry is time dependent, water permeability varies with position along the root and with time. Root water uptake is most effective in young root material, but the length of young roots is not directly related to total root length. In addition, experimental evaluation of root properties is hardly practical, and often impossible. Thus, instead of considering water flow to single roots, a more suitable approach might be the macroscopic one, in which a sink term S representing water extraction by a homogeneous and isotropic element of the root system (volume of water per volume of soil per unit of time) is added to the conservation of mass equation. As it seems to be impossible and unpractical to look for a complete physical description of water extraction by roots, Feddes et al. (1988) described S semi-empirically by:

$$S(h_m) = \alpha(h_m)\, S_{max} \quad \text{... (6)}$$

where $\alpha(h_m)$ is a dimensionless prescribed function of pressure head and S_{max} is the maximal possible water extraction by roots. In the interest of practicality, a homogeneous root distribution can be assumed over the soil profile and define S_{max} according to

$$S_{max} = \frac{T_p}{|Z_r|} \quad \text{... (7)}$$

where T_p is the potential transpiration rate and $|Z_r|$ is the depth of the root zone.

4.3 Groundwater Recharge

There are two types of unsaturated zone (or soil-water) models which can be used for groundwater recharge estimation.

1. Water-balance models
2. Numerical models based on the Richards equation

The literature about practical applications of various types of models for assessing groundwater recharge is limited and does not contain straightforward recommendations about which type of model should be used under different conditions. It is commonly considered that Richards equation-based models are the most theoretically proven and allow to represent flow processes in the porous medium more realistically than water-balance models. However, large-scale applications of Richards equation-based models to highly heterogeneous soils with variable hydraulic properties can be difficult and expensive.

A number of studies have used numerical models to solve Richards' equation for assessing groundwater recharge. A review of previous studies indicate that unit-gradient and fixed water table lower boundary conditions have been applied to models of both constant and variable vertical grid spacing (discretization). It is also reported that whenever the unsaturated flow modelling approach is used to estimate groundwater recharge, a fixed-head lower boundary condition should be selected because it also allows upward flux from the water table during dry periods, a situation that prevails on both sub-humid and semi-arid areas, where accurate groundwater recharge estimates are needed the most. The use of a fixed water table is a simple representation of the regional water table, which in reality interacts with the regional groundwater flow and surface water bodies (e.g., lakes and wetlands).

The use of a variable discretization at the points where both the wetting and drying fronts fluctuate (i.e., top and bottom of soil columns) improve simulation efficiency for the nonlinear unsaturated flow regime. The adequate selection of discretization and boundary conditions, which affect the simulation time, is of utmost importance when a large number of simulations is required (e.g., analysis of climate change scenarios).

5.0 MODELLING OF SOLUTE TRANSPORT THROUGH UNSATURATED ZONE:-

Transport of dissolved solutes in soils is commonly described by the advection-dispersion equation. Prediction of solute migration under field conditions requires the simultaneous solution of the unsaturated flow and solute transport equations. First approximations involve or assume steady flow and constant water contents. Because of the natural complexity of unsaturated flow, methods of predicting solute transport have relied largely on finite difference or finite element approximations of the governing equations.

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.

6.0 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. specified pressure heads or fluxes, and free drainage), models developed recently can cope with much more complex system-dependent boundary conditions evaluating surface flow and energy balances and accounting for the simultaneous movement of water, vapor, and heat. There are also composite models which simulate the processes both in unsaturated and saturated zones and other components of 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.

7.0 CONCLUDING REMARKS:-

Predicting water flow and contaminant transport on a field-scale based on the current monitoring and modelling techniques is a challenging task. There are large uncertainties in predictions mainly due to our inability to depict detailed spatial distributions of soil hydraulic properties on the field-scale. Due to the high costs of data acquisition, few field measurements are usually available for characterization of flow and contaminant transport, even though the spatial distribution of a contaminant plume may be highly irregular. Also, more research associated with water flow and contaminant transport in the unsaturated zone of aquifers containing fractures and karstic conduits is needed for future investigations.

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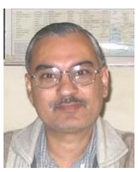

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