

MODELLING OF UNSATURATED FLOW

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Synopsis

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 ground water storage. A fair description of the flow in the unsaturated zone is crucial for predictions of the movement of pollutants into ground water aquifers. 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. The formulation and solution of unsaturated flow problems very often require the use of indirect methods of analysis, based on approximations or numerical techniques. In this paper, various discretization schemes have been presented for modelling of unsaturated flow.

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 overlying 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.

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, interstorm 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 Soil Water Flow

The one-dimensional partial differential equation which describes the movement of moisture through unsaturated porous media subject to appropriate boundary and initial conditions has many field applications in the water environment. In hydrology, it describes the infiltration process that links the surface and sub-surface waters on land. In soil physics, it describes the capillary rise as well as drainage and evaporation of moisture in soils. In environmental pollution, it describes the longitudinal dispersion of pollutants in water courses. Therefore, the problem of seeking solutions to this equation has become a subject of concern for investigators from many different disciplines.

Downward infiltration into an initially unsaturated soil generally occurs under the combined influence of suction and gravity gradients. As the water penetrates deeper and the wetted part of the profile lengthens, the average suction gradient decreases, since the overall difference in pressure head (between the saturated soil surface and the unwetted soil inside the profile) divides itself along an ever-increasing distance. This trend continues until eventually the suction gradient in the upper part of the profile becomes negligible, leaving the constant gravitational gradient in effect as the only remaining force moving water downward. Since the gravitational head gradient has the value of unity (the gravitational head decreasing at the rate of 1 cm with each centimeter of vertical depth below the surface), it follows that the flux tends to approach the hydraulic conductivity as a limiting value. In a uniform soil (without crust) under prolonged ponding, the water content of the wetted zone approaches saturation. However, in practice, because of air entrapment, the soil-water content may not attain total saturation but some maximal value lower than saturation which has been called 'satiation'. Total saturation is assured only when a soil sample is wetted under vacuum.

The dynamics of soil water is cast in the form of mathematical expressions that describe the hydrological relations within the system. The governing equations define a mathematical model. The entire model has usually the form of a set of partial differential equations, together with auxiliary conditions. The auxiliary conditions must describe the system's geometry, the system parameters, the boundary conditions and, in case of transient flow, also the initial conditions. Operations with such a mathematical model are called simulation.

If the governing equations and auxiliary conditions are simple, an exact analytical solution may be found. Otherwise, a numerical approximation is applicable. The numerical simulation models are by far the most applied ones.

Constitutive Equations

The relationships that govern the flow of water in unsaturated soil are quasilinear equations of the parabolic type. Since the coefficients in these equations are functions of the dependent variables, exact analytical solutions for specific boundary conditions are extremely difficult to obtain.

Darcy's equation for vertical flow is

$$q = -K \frac{\partial H}{\partial z} = -K \frac{\partial}{\partial z}(h - z) \quad \dots (1)$$

where q is the flux, H the total hydraulic head, h the soil water pressure head, z the vertical distance from the soil surface downward (i.e., the depth), and K the hydraulic conductivity. At the soil surface, $q = i$, the infiltration rate. In an unsaturated soil, h is negative. Combining this formulation of Darcy's equation (1) with the continuity equation $\partial\theta/\partial t = -\partial q/\partial z$ gives the general flow equation

$$\frac{\partial\theta}{\partial t} = \frac{\partial}{\partial z} \left(K \frac{\partial H}{\partial z} \right) = \frac{\partial}{\partial z} \left(K \frac{\partial h}{\partial z} \right) - \frac{\partial K}{\partial z} \quad \dots (2)$$

If soil moisture content θ and pressure head h are uniquely related, then the left-hand side of equation (2) can be written

$$\frac{\partial\theta}{\partial t} = \frac{d\theta}{dh} \cdot \frac{\partial h}{\partial t}$$

which transforms equation (2) into

$$C \frac{\partial h}{\partial t} = \frac{\partial}{\partial z} \left(K \frac{\partial h}{\partial z} \right) - \frac{\partial K}{\partial z} \quad \dots (3)$$

where $C (= d\theta/dh)$ is defined as the specific (or differential) water capacity (i.e., the change in water content in a unit volume of soil per unit change in matric potential).

Alternatively, we can transform the right-hand side of equation (2) once again using the chain rule to render

$$\frac{\partial h}{\partial z} = \frac{dh}{d\theta} \cdot \frac{\partial \theta}{\partial z} = \frac{1}{C} \cdot \frac{\partial \theta}{\partial z}$$

We thus obtain

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z} \left(\frac{K}{C} \cdot \frac{\partial \theta}{\partial z} \right) - \frac{\partial K}{\partial z}$$

or
$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z} \left(D \cdot \frac{\partial \theta}{\partial z} \right) - \frac{\partial K}{\partial z}$$

...(4)

where D is the soil water diffusivity. Equations (2), (3) and (4) can all be considered as forms of the Richards equation.

Note that the above three equations contain two terms on their right-hand sides, the first term expressing the contribution of the suction (or wetness) gradient and the second term expressing the contribution of gravity. Whether the one or the other term predominates depends on the initial and boundary conditions and on the stage of the process considered. For instance, when infiltration takes place into an initially dry soil, the suction gradients at first can be much greater than the gravitational gradient and the initial infiltration rate into a horizontal column tends to approximate the infiltration rate into a vertical. On the other hand, when infiltration takes place into an initially wet soil, the suction gradients are small from the start and become negligible much sooner. The effects of ponding depth and initial wetness can be significant during early stages of infiltration, but decrease in time and eventually tend to vanish in a very deeply wetted profile.

The following simplifications can be introduced to find analytical solutions: K is an analytical function of θ or h ; hysteresis is neglected; the medium is homogeneous and isotropic; the flow is considered to be stationary or a succession of steady-state situations (quasistationary approach); the gravity force is neglected. The first two assumptions linked with the third one have resulted in a great number of analytical solutions. The gravity force is often neglected in describing the infiltration process in originally dry soil, resulting in analytical solutions as derived by e.g. Philip (1957, 1958).

The classical Richards-flow theory (Richards, 1931), upon which most simulation models are based, holds for stable flow conditions only. Yet instability of flow has been observed under a wide variety of circumstances such as abrupt and gradual increases of hydraulic conductivity with depth, compression of air ahead of the wetting front and water repellency of the solid phase. Another example of non-Richards type of flow is the preferential flow through non-capillary macropores. With classical flow theories one may then underestimate the velocity and depth of water/solute transport.

3.0 Numerical Approach

With the advance of digital computers, emphasis has shifted drastically from the classical approach of analytical solutions to the rapidly developing field of numerical analysis. At present, numerical approximations are possible for complex, compressible, nonhomogeneous and anisotropic flow regions having various boundary configurations.

Numerical methods are based on subdividing the flow region into finite segments bounded and represented by a series of nodal points at which a solution is obtained. This solution depends on the solutions of the surrounding segments and on an appropriate set of auxiliary conditions. In recent years, a number of numerical methods have been introduced. The methods most appropriate to the problem of soil water dynamics

are finite difference method, finite element method and boundary element method. The finite difference method has been discussed below.

3.1 Finite Difference Methods

Finite difference methods (Remson et al., 1971), either explicit or implicit, belong to the most frequently used techniques in modelling unsaturated flow conditions. The most simple type of finite differencing, the explicit one, orders the differencing operators in such a manner that the resulting finite difference equation contains only one unknown, and consequently, may be solved simply and directly. The explicit method is computationally simple but it has one serious drawback. In order to attain reasonable accuracy, the length of the interval in space must be kept small. To get a stable solution, the time step has to be small compared with the space interval. Thus, it is necessary to have a large number of time steps when using the simple explicit method.

Implicit solution methods generally use much larger time steps than explicit ones, but their stability depends upon the degree of nonlinearity of the differential equation. There are a great number of methods to solve an implicit set of algebraic equations, such as linearization, predictor-corrector or iteration methods.

In dealing with unsaturated flow problems that involve more than one space dimension and a grid with many nodal points, it is often necessary to use a mixed scheme that relies on simultaneous displacements along one space dimension and on successive displacements along the remaining space dimensions. This leads to the method of successive over relaxation (SOR). In the case of isotropic conditions, faster convergence may be sometimes achieved by using the iterative alternating direction implicit procedure (ADIPIIT).

The advantage of the finite difference method is its simplicity and efficiency in treating the time derivatives. On the other hand, the method is rather incapable to deal with complex geometries of flow regions. A slow convergence, a restriction to bilinear grids and difficulties in treating moving boundary conditions are other serious drawbacks of the method.

3.2 Discretization Schemes

Different discretization schemes can be used using explicit or implicit methods. In the explicit method, a series of linearized independent equations is solved directly, while in the implicit method, a system of simultaneous linear algebraic equations (involving tridiagonal coefficient matrix with zero elements outside the diagonals) has to be solved. For a given grid point at a given time, the values of the coefficients $K(h)$ or $K(\theta)$ and $C(h)$ or $D(\theta)$ can be expressed either from their values at the preceding time step (explicit linearization) or from a prediction at time $(t+1/2\Delta t)$ using a method described by Douglas and Jones, 1963 (implicit linearization).

The following discretization schemes (Equation 3) can be used for the various models.

Model 1 : Explicit Scheme Solved Directly

$$h_i^{j+1} = h_i^j + \frac{\Delta t}{C_i^j \Delta z} \left[K_{i+1/2}^j \left(\frac{h_{i+1}^j - h_i^j}{\Delta z} - 1 \right) - K_{i-1/2}^j \left(\frac{h_i^j - h_{i-1}^j}{\Delta z} - 1 \right) \right] \quad \dots (5)$$

where, j refers to time, and i refers to depth and

$$K_{i+1/2}^j = \frac{K_{i+1}^j + K_i^j}{2};$$

$$K_{i-1/2}^j = \frac{K_i^j + K_{i-1}^j}{2}.$$

Defining D_{\max} as the maximum value of the soil water diffusivity in the soil profile at time t, the scheme is stable when (Haverkamp et al., 1977)

$$\Delta t < \frac{r(\Delta z)^2}{D_{\max}} \quad \dots (6)$$

where, ΔZ is the layer thickness and r an arbitrary chosen coefficient.

The method is limited by extensive use of computer time when the water content approaches saturation and Δt becomes very small (D_{\max} becomes large).

Model 2 : Implicit Scheme with Explicit Linearization

$$C_i^j \frac{h_i^{j+1} - h_i^j}{\Delta t} = \frac{1}{\Delta z} \left[K_{i+1/2}^j \left(\frac{h_{i+1}^{j+1} - h_i^{j+1}}{\Delta z} - 1 \right) - K_{i-1/2}^j \left(\frac{h_i^{j+1} - h_{i-1}^{j+1}}{\Delta z} - 1 \right) \right]$$

or

$$C_i^j \frac{h_i^{j+1} - h_i^j}{\Delta t} = \frac{1}{\Delta z} \left[\left(\frac{K_{i+1}^j + K_i^j}{2} \right) \left(\frac{h_{i+1}^{j+1} - h_i^{j+1}}{\Delta z} - 1 \right) - \left(\frac{K_i^j + K_{i-1}^j}{2} \right) \left(\frac{h_i^{j+1} - h_{i-1}^{j+1}}{\Delta z} - 1 \right) \right]$$

Rearranging the terms, we get

$$\left[-F_2 \frac{\Delta t}{(\Delta z)^2} \right] h_{i-1}^{j+1} + \left[C_i^j + (F_1 + F_2) \frac{\Delta t}{(\Delta z)^2} \right] h_i^{j+1} - \left[F_1 \frac{\Delta t}{(\Delta z)^2} \right] h_{i+1}^{j+1} = C_i^j h_i^j + (F_2 - F_1) \frac{\Delta t}{\Delta z} \quad \dots (7)$$

where,

$$F_1 = K_{i+1/2}^j = \frac{K_{i+1}^j + K_i^j}{2};$$

$$F_2 = K_{i-1/2}^j = \frac{K_i^j + K_{i-1}^j}{2}.$$

Model 3 : Implicit Scheme with Implicit Linearization (Prediction - Correction)

From equation (3), we have

$$C \frac{\partial h}{\partial t} = \frac{\partial}{\partial z} \left[K \left(\frac{\partial h}{\partial z} - 1 \right) \right]$$

or

$$C \frac{\partial h}{\partial t} = \frac{\partial K}{\partial z} \left(\frac{\partial h}{\partial z} - 1 \right) + K \frac{\partial^2 h}{\partial z^2}$$

or

$$\frac{C}{K} \frac{\partial h}{\partial t} = \frac{\partial^2 h}{\partial z^2} + \frac{1}{K} \frac{\partial K}{\partial z} \left(\frac{\partial h}{\partial z} - 1 \right) \quad \dots (8)$$

Prediction (Estimation of C_i^j and K_i^j):

From equation (8), by taking time step as $\Delta t/2$, we have

$$\frac{2C_i^j}{K_i^j} \cdot \frac{h_i^{j+1/2} - h_i^j}{\Delta t} = \frac{h_{i+1}^{j+1/2} - 2h_i^{j+1/2} + h_{i-1}^{j+1/2}}{(\Delta z)^2} + \frac{1}{K_i^j} \cdot \frac{K_{i+1}^j - K_{i-1}^j}{2\Delta z} \left[\frac{h_{i+1}^j - h_{i-1}^j}{2\Delta z} - 1 \right]$$

Rearranging the terms, we get

$$-\frac{\Delta t}{(\Delta z)^2} h_{i-1}^{j+1/2} + \left[\frac{2C_i^j}{K_i^j} + \frac{2\Delta t}{(\Delta z)^2} \right] h_i^{j+1/2} - \frac{\Delta t}{(\Delta z)^2} h_{i+1}^{j+1/2} = \frac{2C_i^j}{K_i^j} h_i^j + \frac{1}{2} \frac{K_{i+1}^j - K_{i-1}^j}{K_i^j} \frac{\Delta t}{\Delta z} \left[\frac{h_{i+1}^j - h_{i-1}^j}{2\Delta z} - 1 \right]$$

... (9)

Correction (Estimation of h_i^j):

From equation (8), by taking time step as Δt , we have

$$\frac{C_i^{j+1/2}}{K_i^{j+1/2}} \cdot \frac{h_i^{j+1} - h_i^j}{\Delta t} = \frac{1}{2} \left[\frac{h_{i+1}^{j+1} - 2h_i^{j+1} + h_{i-1}^{j+1}}{(\Delta z)^2} + \frac{h_{i+1}^j - 2h_i^j + h_{i-1}^j}{(\Delta z)^2} \right] + \frac{1}{K_i^{j+1/2}} \cdot \frac{K_{i+1}^{j+1/2} - K_{i-1}^{j+1/2}}{2\Delta z} \left[\frac{h_{i+1}^{j+1/2} - h_{i-1}^{j+1/2}}{2\Delta z} - 1 \right]$$

Rearranging the terms, we get

$$-\frac{1}{2} \frac{\Delta t}{(\Delta z)^2} h_{i-1}^{j+1} + \left[\frac{C_i^{j+1/2}}{K_i^{j+1/2}} + \frac{\Delta t}{(\Delta z)^2} \right] h_i^{j+1} - \frac{1}{2} \frac{\Delta t}{(\Delta z)^2} h_{i+1}^{j+1}$$

$$= \frac{C_i^{j+1/2}}{K_i^{j+1/2}} h_i^j + \frac{1}{2} \frac{\Delta t}{(\Delta z)^2} [h_{i+1}^j - 2h_i^j + h_{i-1}^j] + \frac{1}{2} \frac{K_{i+1}^{j+1/2} - K_{i-1}^{j+1/2}}{K_i^{j+1/2}} \frac{\Delta t}{\Delta z} \left[\frac{h_{i+1}^{j+1/2} - h_{i-1}^{j+1/2}}{2\Delta z} - 1 \right]$$

... (10)

Model 4 : Crank-Nicolson Scheme

$$C_i^{j+1/2} \frac{h_i^{j+1} - h_i^j}{\Delta t} = \frac{1}{\Delta z} \left[K_{i+1/2}^{j+1/2} \left(\frac{h_{i+1}^{j+1/2} - h_i^{j+1/2}}{\Delta z} - 1 \right) - K_{i-1/2}^{j+1/2} \left(\frac{h_i^{j+1/2} - h_{i-1}^{j+1/2}}{\Delta z} - 1 \right) \right]$$

where,

$$h_i^{j+1/2} = \frac{h_i^j + h_i^{j+1}}{2};$$

$$K_{i-1/2}^{j+1/2} = F_1 = \left(\frac{K_i^j K_{i-1}^j}{K_i^j + K_{i-1}^j} \right) + \left(\frac{K_i^{j+1} K_{i-1}^{j+1}}{K_i^{j+1} + K_{i-1}^{j+1}} \right)$$

$$K_{i+1/2}^{j+1/2} = F_2 = \left(\frac{K_i^j K_{i+1}^j}{K_i^j + K_{i+1}^j} \right) + \left(\frac{K_i^{j+1} K_{i+1}^{j+1}}{K_i^{j+1} + K_{i+1}^{j+1}} \right)$$

$$C_i^{j+1/2} = F_3 = \frac{C_i^j + C_i^{j+1}}{2}.$$

Rearranging the terms, we get

$$\begin{aligned} & -\frac{1}{2} F_1 \frac{\Delta t}{(\Delta z)^2} h_{i-1}^{j+1} + \left[F_3 + \frac{1}{2} (F_1 + F_2) \frac{\Delta t}{(\Delta z)^2} \right] h_i^{j+1} - \frac{1}{2} F_2 \frac{\Delta t}{(\Delta z)^2} h_{i+1}^{j+1} \\ & = \frac{1}{2} F_1 \frac{\Delta t}{(\Delta z)^2} h_{i-1}^j + \left[F_3 - \frac{1}{2} (F_1 + F_2) \frac{\Delta t}{(\Delta z)^2} \right] h_i^j + \frac{1}{2} F_2 \frac{\Delta t}{(\Delta z)^2} h_{i+1}^j + (F_1 - F_2) \frac{\Delta t}{\Delta z} \\ & \dots (11) \end{aligned}$$

When equation (7), (9), (10) or (11) is applied at all nodes, the result is a system of simultaneous linear algebraic equations with a tridiagonal coefficient matrix with zero elements outside the diagonals and unknown values of h. In solving this system of equations, a so-called direct method can be used by applying a tridiagonal algorithm of the kind discussed by Remson et al. (1971).

3.3 Initial and Boundary Conditions

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

3.3.1 Upper boundary conditions

While the potential evapotranspiration rate from a soil depends only 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 can not 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 $h^{\text{lim}} \leq h \leq 0$, 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 $h = h^{\text{lim}}$. 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).

If the relative humidity (f) and the temperature of the air (T) as a function of time are known, and if it may be assumed that the pressure head at the soil surface is at equilibrium with the atmosphere, then $h(0,t)$ can be derived from the thermodynamic relation (Edlefsen and Anderson, 1943):

$$h(0,t) = \frac{RT(t)}{Mg} \ln[f(t)] \quad \dots (12)$$

where R is the universal gas constant (8.314×10 erg/mole/K), T is the absolute temperature (K), g is acceleration due to gravity (980.665 cm/s²), M is the molecular weight of water (18 gm/mole), f is the relative humidity of the air (fraction) and h is in bars. Knowing $h(0,t)$, $\theta(0,t)$ can be derived from the soil water retention curve.

3.3.2 Lower boundary conditions

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 ground water table, a Neumann type of boundary condition is used.

Dirichlet condition

Easy recording of changes in phreatic surface in case of present ground water table is the main advantage of specifying a matric head zero as the bottom boundary. A drawback is that with shallow ground water tables (less than 2 m below soil surface) the simulated effects of changes in phreatic surface are extremely sensitive to variations in the soil hydraulic conductivity.

The nodal points in a soil profile usually have fixed positions and probably none of them will coincide with the water table level. The nodal point, where the matric head is prescribed, is often the one immediately beneath the phreatic level. When large fluxes across the lower boundary occur, an error is introduced by this approximation.

Neumann condition

A flux as lower boundary condition is usually applied in cases where one can identify a no-flow boundary (e.g. an impermeable layer) or a free drainage case. In the latter case the flux is always directed downward and the gradient $dh/dz = 1$, so the Darcian flux is equal to the hydraulic conductivity at the lower boundary.

Cauchy condition

This type of boundary condition is used when unsaturated flow models are combined with models for regional ground water flow or when the effects of surface water management are to be simulated. Writing the lower boundary flux as function of the phreatic surface, which is in this case the dependent variable, one can incorporate relationships between the flux to/from the drainage system and the height of the phreatic surface. This flux-head relation can be obtained from drainage formulae or from regional ground water flow models.

With the lower boundary conditions, the connection with the saturated zone can be established. In this way, effects of activities influencing the regional ground water system upon, for instance, crop evapotranspiration can be simulated. The coupling between the two systems is possible by considering the phreatic surface as an internal moving boundary with one-way or two-way relationships. When the Cauchy

condition is linked with a one-dimensional vertical flow model, one can consider such a solution as quasi-two-dimensional, since both vertical and horizontal flow are calculated.

4.0 Required Input Data

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, $K(\theta)$.

For a proper description of the unsaturated flow, a correct description of the two hydraulic functions, $K(\theta)$ and $h(\theta)$, is important. The hydraulic conductivity, $K(\theta)$, decreases strongly as the moisture content θ , decreases from saturation. The experimental procedure for measuring $K(\theta)$ at different moisture contents is rather difficult and not very reliable. Alternative procedures have been suggested to derive the $K(\theta)$ function from more easily 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 saturation, and hydraulic conductivity at saturation. The relation is given by

$$K(\theta) = K_s \left(\frac{\theta - \theta_r}{\theta_s - \theta_r} \right)^n \quad \dots (13)$$

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 $h(\theta)$ and moisture content θ , usually termed as the water retention curve or the soil moisture characteristic, is basically 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 may appear, and, instead of being a single valued relationship, the h - θ relation consists of a family of curves. The actual curve will have to be determined from the history of wetting and drying.

If root water uptake is also modelled, the parameters defining the relation between root water uptake and soil water status should be given, together with crop specifications. In case a functional flux-head relationship is used as lower boundary condition, the parameters describing the interaction between surface water and ground water and, if necessary, the vertical resistance of poorly permeable layers have to be supplied.

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