A Mathematical Model for Predicting Isothermal Soil Moisture Profiles Using Finite Difference Method

Kasthurirangan Gopalakrishnan and Anshu Manik

***Abstract*—**Subgrade moisture content varies with environmental and soil conditions and has significant influence on pavement performance. Therefore, it is important to establish realistic estimates of expected subgrade moisture contents to account for the effects of this variable on predicted pavement performance during the design stage properly. The initial boundary soil suction profile for a given pavement is a critical factor in determining expected moisture variations in the subgrade for given pavement and climatic and soil conditions. Several numerical models have been developed for predicting water and solute transport in saturated and unsaturated subgrade soils. Soil hydraulic properties are required for quantitatively describing water and chemical transport processes in soils by the numerical models. The required hydraulic properties are hydraulic conductivity, water diffusivity, and specific water capacity. The objective of this paper was to determine isothermal moisture profiles in a soil fill and predict the soil moisture movement above the ground water table using a simple one-dimensional finite difference model.

***Keywords*—**Fill, Hydraulic Conductivity, Pavement, Subgrade.

I. Introduction

HYDROGEOLOGY is the part of hydrology that deals with the occurrence, movement and quality of water beneath the Earth's surface. Because hydrogeology deals with water in a complex subsurface environment, it is a complex science. On the other hand, much of its basic terminology and principles can be understood readily by non-hydrogeologists [1]. Many terms are used to describe the nature and extent of the groundwater resource. The level below which all the spaces are filled with water is called the *water table*. Above the water table lies the unsaturated zone. Here the spaces in the rock and soil contain both air and water. Water in this zone is called *soil moisture*. The entire region below the water table is called the saturated zone, and water in this saturated zone is called groundwater [2].

Classical soil mechanics has emphasized specific types of soils (e.g., saturated sands, silts, and clays and dry sands). Textbooks cover the theories related to these types of soils in a completely dry or a completely saturated condition. Recently, it has been shown that attention must be given to soils that do not fall into these common categories. Many of these soils can be classified as unsaturated soils. Engineering related to unsaturated soils has typically remained empirical due to the complexity of their behavior [3]. Laboratory studies have shown that there is a relationship between the Soil-Water Characteristic Curve (SWCC) and unsaturated soil properties [4].

The SWCC for a soil is the relationship between the suction, ψ, exhibited by it and its volumetric water content, θ. Many unsaturated soil properties (or soil property functions) can be related to the water content versus suction relationship of a soil. Hydraulic conductivity, shear strength, chemical diffusivity, water storage, unfrozen volumetric water content, specific heat, and thermal conductivity are all functions of the SWCC. Application of SWCC for estimating unsaturated soil hydraulic conductivity [5], shear strength [6], swelling potential [7] and its compressibility [8] is very well established.

The coefficient of permeability or hydraulic conductivity, K, of an unsaturated soil is not a constant. The coefficient of permeability depends on the volumetric water content θ, which, in turn, depends upon the soil suction, ψ. The soil suction may be either the matric suction of the soil, (i.e., u_a-u_w, where u_a is pore-air pressure, and u_w is pore-water pressure), or the total suction (i.e., matric plus osmotic suctions). Soil suction is one of the two stress state variables that control the behavior of unsaturated soils [10].

The solution of the linear partial differential equation of flow was first proposed by Casagrande [11] through the use of the graphical flownet method. This method is based on the assumptions that the soil is homogenous and isotropic, and that water flows only in the saturated zone. The boundaries of the flow region must be defined in terms of head or no-head flow. The flownet solutions proposed by Casagrande [11] were for simple unconfined flow cases without flux boundary conditions. In the late 1960's, the development and application of digital computer to solving complex seepage problems came into prominence. Freeze [12] proposed a finite difference model of flow through both the saturated and

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unsaturated soil regions. In the late 1970s, the increased computer power, combined with the finite element method became a powerful tool in solving steady state and transient saturated-unsaturated seepage problems [13].

Many equations describing the soil water characteristic appear in the literature. Recently, Dourado-Neto et al. [14] developed computer software for 12 analytical models in the literature to describe the soil water characteristic. The most universally used model, published by van Genuchten [5], is applicable to S-shaped relationships, while that of Brooks and Corey [15] is applicable to C-shaped relationships. A special feature of both models is the introduction of the concept of the residual water content θ_r, which is approached asymptotically by both models [16].

The objective of this paper is to determine isothermal moisture profiles in a soil fill and predict the soil moisture movement above the ground water table through the use of explicit finite difference modeling. Although several numerical models are now available in the form of computer software to accomplish this, this paper is intended to demonstrate the steps involved in developing such computational models which would be greatly helpful for educators and students. The methodology is demonstrated by taking an example of a soil fill to be constructed in Northern Illinois.

II. Theory

Measurement of the hydraulic conductivity of soil, *K*, can be made either in the laboratory or in the field by using different methods, which often have different operating ranges, flow geometries, boundary conditions, sample sizes, and underlying assumptions. Selecting the proper method for particular soil and site conditions, and the proper application procedure for the selected method, is important to obtain representative estimates of *K* [17]. Numerous attempts have been made to predict empirically the hydraulic conductivity function for an unsaturated soil. These procedures make use of the saturated coefficient of permeability and the SWCC for the soil. As more precise equations have been developed for the soil-water characteristic curve, likewise, more reliable predictions have been made for the hydraulic conductivity function.

Soil hydraulic properties are required for quantitatively describing water and chemical transport processes in soils by the numerical models. Soil water diffusivity, *D*, is one of the important hydraulic properties. In recent years, there have been increased efforts to estimate soil water diffusivities of unsaturated soils, as one of the major soil hydraulic properties [18].

Usually horizontal infiltration experiments have been used to relate soil water diffusivity to the volumetric water content by the method of [19]. The method is based on the Boltzmann transformation. The slope of the water content distribution curve along the soil column needs to be measured to estimate the water diffusivity. This common method for estimating soil water diffusivity is described in detail by [20]. However, it is difficult to exactly determine the slope of the water content distribution curve which leads to soil water diffusivity estimation error.

Cassel et al. [21] presented a method for estimating soil water diffusivity from time-dependent soil water content distributions in the horizontal redistribution process. Their method requires measuring water content distribution with time and also involves both relatively intensive calculation and time-consuming experiments. Clothier et al. [22] presented a fitting function chosen from those presented by Philip [23] to approximate the water distribution curve in the [19] method. This made possible a simple analytical expression of the water diffusivity by avoiding finding the slopes of the soil water distribution curve [18].

Shao and Horton [24] assumed a power function between the soil water diffusivity and the soil water content, however the form of their power function may not apply to all soils. A power function relationship between soil water diffusivity and relative water content may have a more general application to soils than does the Shao and Horton [24] power function relationship.

Darcy's equation describing one-dimensional horizontal flow of water in unsaturated soil is:

$$q = K(\theta)\frac{\Delta h}{\Delta L} = K(\theta)\frac{\partial h}{\partial z} = -D(\theta)\frac{\partial \theta}{\partial z} \tag{1}$$

And the continuity equation is:

$$\frac{\partial \theta}{\partial t} = -\nabla q \tag{2}$$

where q is soil water flux, $K(\theta)$ is unsaturated hydraulic conductivity, h is soil–water suction, x is the horizontal distance (cm), $D(\theta)$ is the soil water diffusivity, and θ is the soil water content.

The following equation was used to describe the unsaturated hydraulic conductivity [15]:

$$K(h) = K_s\left(\frac{h_d}{h}\right)^m \tag{3}$$

where K_s is saturated conductivity, h_d is air-entry suction, and m is a constant.

Passioura [25] developed a method of calculating diffusivity from one-step outflow data and his method is adopted here. The method is based on the assumption that the rate of change of water content at any time is effectively uniform throughout the draining column of the soil (i.e. $\partial\theta/\partial t$ is assumed constant throughout the soil column; θ is volumetric soil content and t is time). This makes the solution of diffusion equation simpler than other approaches [26].

With the one-step method, a pressure is applied at the upper end (z = L, where L is the length of the soil column) of a soil sample with an initial water content, θ_i. The outflow is then measured at the lower end, z = 0, where it is assumed that water content is reduced to the final water content (θ_f) at the onset of the outflow. The governing equation, neglecting gravity, and the initial and boundary conditions are as follows:

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}\left(D \frac{\partial \theta}{\partial z} \right) \tag{4}$$

$$\theta(x,0) = \theta_i$$
$$\theta(0,t) = \theta_s$$
$$\theta(\infty,t) = \theta_i \tag{5}$$

where θ_i is the initial soil water content. Integrating Eq. [3] with respect to θ gives:

$$\int_{\theta}^{\theta_s} \frac{\partial z}{\partial t} d\theta + D(\theta_s)\left[\frac{\partial \theta}{\partial z}\right]_s - D(\theta)\frac{\partial \theta}{\partial z} = 0 \tag{6}$$

Parlange [27] considered that the first term in Eq. [6] is small compared with the rest of the terms in Eq. [6] and may be neglected when soil water content is close to the saturated water content. Eq. [6] reduces to:

$$D(\theta_s)\left[\frac{\partial \theta}{\partial z}\right]_s \approx D(\theta)\frac{\partial \theta}{\partial z} \tag{7}$$

Using the definition of diffusivity [28], soil water diffusivity can be be expressed as a function of soil water retention curve and unsaturated soil water conductivity curve:

$$D = -K\frac{dh}{d\theta} \quad \text{or} \quad D(\theta) = K(\theta)\frac{dh}{d\theta} \tag{8}$$

Therefore,

$$D(\theta) = K(\theta)\frac{\Delta h}{\Delta \theta} \tag{9}$$

III. Finite Difference Formulation

As mentioned previously, the objective of this paper is to determine isothermal moisture profiles in a soil fill and predict the soil moisture movement above the ground water table through the use of explicit finite difference modeling. The methodology is demonstrated through a real-world example.

A 4-ft. high fill of Fayette C soil is to be constructed in Northern Illinois at a dry density of 101.1 pcf and optimum gravimetric water content of 17%. Prior to constructing the 4-ft fill, 1 ft. of soil will be stripped away because of high organic content. The water table is very close to the surface in this soil and it was found to be saturated at the starting grade after the 1 ft. of soil was excavated. It is required to determine the isothermal moisture profile in the 4 ft. of Fayette C fill (now 5 ft. thick) after 3 days and 6 days. It is also required to determine the time duration (days) for the fill at a location 1 ft. below the surface to reach equilibrium water content.

The Soil-Water Characteristic Curve (SWCC) is used to represent the relationship between volumetric water content, θ, and matric suction. Using the SWCC (i.e., desorption curve) for Fayette C soil (see Fig. 1), the gravimetric water contents were converted to volumetric water contents. Gravimetric water content is the weight of soil water per unit weight of dry soil, whereas volumetric water content is the volume of soil water per unit of total volume.

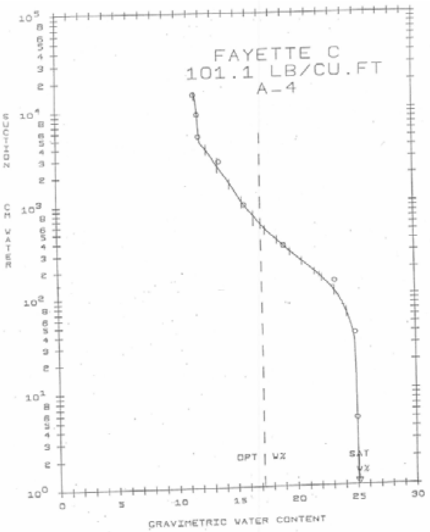

Fig. 1 Suction curve for Fayette C soil

Numerous empirical equations have been proposed to simulate the SWCC. Each equation appears to apply for a particular group of soils. There are other equations of slightly differing forms that could be tested to assess their fit with experimental data. For example, the SWCC appears to have the form of the right-hand side of a normal-distribution curve [9]. Among the earliest is an equation proposed by Brooks and Corey [15]. It is in the form of a power-law relationship:

$$\theta = \left(\frac{\psi_b}{\psi}\right)^{\lambda} \tag{10}$$

where θ = normalized (or dimensionless) water content; ψ = suction; ψ_b = air-entry value; and λ = pore-size distribution index.

The following linear relationship between the logarithm of volumetric water content and the logarithm of suction was used by Williams et al. [29] to describe the SWCC of many soils in Australia (a_1 and b_1 are curve-fitting parameters):

$$\ln\psi = a_1 + b_1 \ln\theta \tag{11}$$

Volumetric and gravimetric water content are related by the bulk density of the soil through the following relation:

$$\theta = w\left(\frac{\rho_{soil}}{\rho_{water}}\right) \tag{12}$$

where w is the gravimetric water content and θ is the volumetric water content; ρ_{soil} is the density of soil and ρ_{water} is the density of water. By substituting a value of 101.1 lb/ft^3 (for Fayette C soil) for ρ_{soil} and 62.4 lb/ft^3 for ρ_{water}, Eq. [10] can be written as:

$$\theta = w\left(\frac{101.1}{62.4}\right) \tag{13}$$

To determine the rate of soil moisture movement above the ground water table, either an implicit or explicit finite difference formulation could be used. In this study, an explicit finite difference formulation is used. The first step is to obtain mathematical models for *K(θ)* versus θ and *D(θ)* versus θ relations which would be used in the finite difference solution.

Using the hydraulic conductivity function curve for Fayette C soil (i.e. *K(θ)* versus θ curve) (see Fig. 2), representative θ values and the corresponding *K(θ)* values were selected. Regression analysis was conducted to derive a model which predicts *K(θ)* as a function of θ. Gardner [30] proposed an equation for the hydraulic conductivity function. The equation emulates the soil-water characteristic curve and is written as follows:

$$\theta = \frac{1}{1 + q\psi^n} \tag{14}$$

where q is a curve-fitting parameter related to the air-entry value of the soil, and n is a curve-fitting parameter related to the slope at the inflection point on the soil-water characteristic curve.

In this study, the following relation was obtained between *K(θ)* and θ for Fayette C soil:

$$K(\theta) = 1302.32 * \theta^{13.769}$$
$$R^2 = 0.993; SEE = 0.133 \tag{15}$$

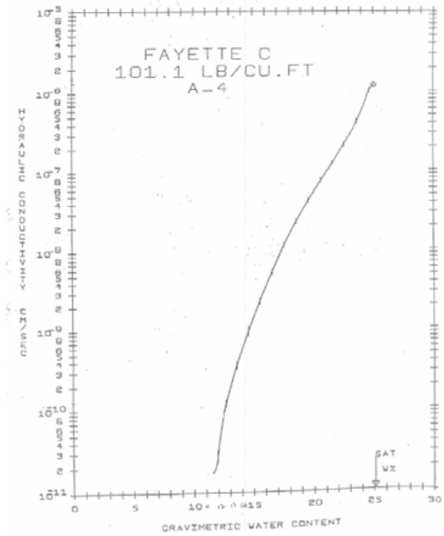

Fig. 2 Hydraulic conductivity versus gravimetric water content for Fayette C soil

Similarly, using the SWCC for Fayette C soil together with the hydraulic conductivity curve, a regression model for *D(θ)* as a function of θ was obtained using the relation between *K(θ)* and *D(θ)*:

$$D(\theta) = \frac{\Delta h}{\Delta\theta} K(\theta_{mid}) \tag{16}$$

The following relation was obtained between *D(θ)* and θ for Fayette C soil:

$$D(\theta) = 4.26E - 04 * e^{25.275\theta} \tag{17}$$

Later on, it was found that the mathematical model used for *D(θ)* significantly affects the shape of the isothermal moisture profiles and the duration for the fill at various depths below the surface to reach equilibrium water contents. When using the *Exponential* model (Eq. [17]) for *D(θ)*, it was found that the water content at 20 cm below the surface becomes lower than the optimum water content and this trend became pronounced with increasing time duration (see Fig. 3). This problem was rectified by using a *Power* model for *D(θ)* which gave similar R^2 and Standard Error of Estimate (SEE) values:

$$D(\theta) = 8070 * \theta^{7.50}$$
$$R^2 = 0.910; SEE = 0.225 \tag{18}$$

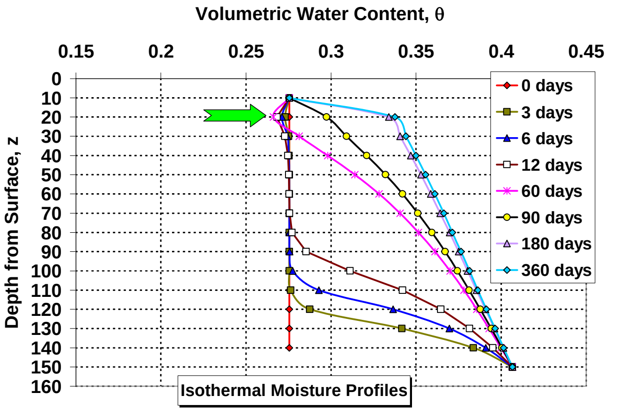

Fig. 3 Isothermal misture pofiles otained uing the Exponential mdel for $D(\theta)$ in the Finite Difference slution. The problem area is shown using arrow. Because of this the Exponential model was replaced by the Power model

A generalized program was created in *Visual Basic* programming language to implement the explicit finite difference formulations (see Fig. 4). The steps involved in the finite difference formulation are as follows.

The general equation relating hydraulic conductivity and diffusivity to volumetric water content is described as:

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}[D(\theta)\frac{\partial \theta}{\partial z}] + \frac{\partial K(\theta)}{\partial z} \tag{19}$$

In explicit finite difference form, Eq. [19] can be written as:

$$\frac{\theta_j^{n+1} - \theta_j^n}{\Delta t} = \frac{D(\theta_{j+1/2}^{n+1/2}) * \frac{(\theta_{j+1}^n - \theta_j^n)}{\Delta z} - D(\theta_{j-1/2}^{n+1/2}) * \frac{(\theta_j^n - \theta_{j-1}^n)}{\Delta z}}{\Delta z} + \frac{K(\theta_{j+1/2}^{n+1/2}) - K(\theta_{j-1/2}^{n+1/2})}{\Delta z} \tag{20}$$

where n is the time step and j is the node. The individual terms in Eq. [20] could be substituted using the following equations:

$$D(\theta) = K(\theta)\frac{\partial h}{\partial \theta} \tag{21}$$

$$D(\theta_{j+1/2}^{n+1/2}) = D(\theta_{j+1/2}^*) \tag{22}$$

$$K(\theta_{j+1/2}^{n+1/2}) = K(\theta_{j+1/2}^*) \tag{23}$$

$$D(\theta_{j+1/2}^*) = \sqrt{D(\theta_j) * D(\theta_{j+1})} \tag{24}$$

$$K(\theta_{j+1/2}^*) = \sqrt{K(\theta_j) * K(\theta_{j+1})} \tag{25}$$

$$D(\theta_{j-1/2}^{n+1/2}) = D(\theta_{j-1/2}^*) \tag{26}$$

$$K(\theta_{j-1/2}^{n+1/2}) = K(\theta_{j-1/2}^*) \tag{27}$$

$$D(\theta_{j-1/2}^*) = \sqrt{D(\theta_{j-1}) * D(\theta_j)} \tag{28}$$

$$K(\theta_{j-1/2}^*) = \sqrt{K(\theta_{j-1}) * K(\theta_j)} \tag{29}$$

The iterations were performed at Δz = 10 cm with small time steps of about 1.0 hr. The implemented program for explicit finite difference formulation has a user interface through which the user can input the values for dry density, saturated gravimetric water content, optimum gravimetric water content, total analysis depth, total height of the soil column, the depth increment and the time step (see Fig. 4).

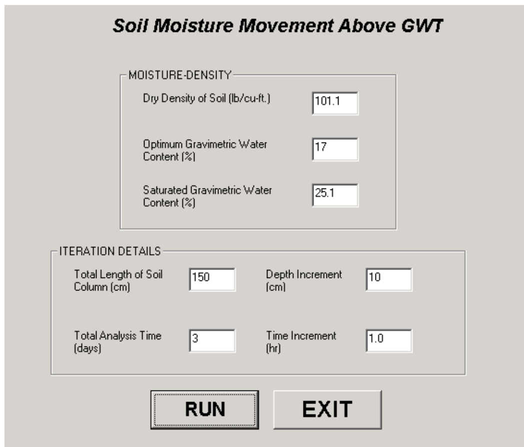

Fig. 4 Visual Basic user-interface for explicit finite difference model implementation to predict soil moisture movement above ground water table for Fayette C soil

An output file is created which contains the values of the volumetric water content (θ) at every node and at every time step during the iteration. Using this information, isothermal moisture profiles in the 5 ft. of Fayette C fill after 3 days and 6 days were determined (see Fig. 5). Note that the initial condition (0 days) is that the bottommost node which is in contact with the water table is assigned the saturated volumetric water content (**θ_{sat} = 0.406 cm^3/cm^3**) and all other nodes are assigned the optimum volumetric water content (**θ_{opt} = 0.275**). As time progresses, the soil would "wet-up" because of suction.

To determine how long it will take for the fill at a location 1 ft. (30 cm) below the surface to reach equilibrium water content, the program was run at different time durations: 3, 6, 12, 48, 60, 90, 180, 360 days, etc. By plotting the volumetric water contents at 1 ft. (obtained from the corresponding node) below the surface against time (days), the time to reach equilibrium water content was obtained (see Fig. 6).

The equilibrium (volumetric) water content for the fill at a location 1 ft. below the surface is *0.356*. The equilibrium water contents at various depths could also be obtained using the suction curve for Fayette C soil. Using the suction curve, a value of *0.38* is obtained. It would take approximately *180 days* to reach the equilibrium water content.

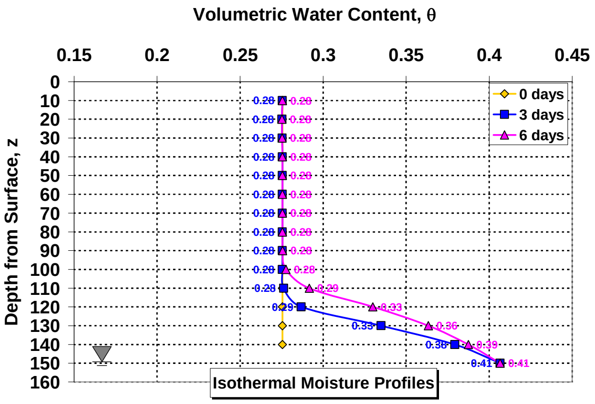

Fig. 5 Development of isothermal moisture profiles

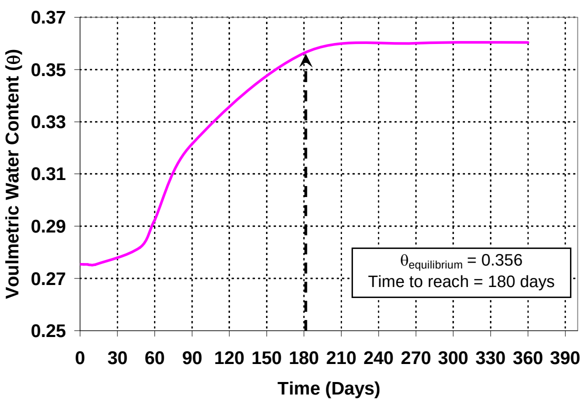

Fig. 6 Time to reach equilibrium water content at a location 1 ft. below the surface of Fayette C soil fill

IV. Conclusions

The initial boundary soil suction profile for a given pavement is a critical factor in determining expected moisture variations in the subgrade for given pavement and climatic and soil conditions. Several numerical models have been developed for predicting water and solute transport in saturated and unsaturated soils. Soil hydraulic properties are required for quantitatively describing water and chemical transport processes in soils by the numerical models. The required hydraulic properties are hydraulic conductivity, water diffusivity, and specific water capacity. Among the three parameters, only two of them are independent.

The Soil-Water Characteristic Curve (SWCC) is used to represent the relationship between volumetric water content and matric suction. Numerous empirical equations have been proposed to simulate the SWCC. Each equation appears to apply for a particular group of soils. There are other equations of slightly differing forms that could be tested to assess their fit with experimental data. The objective of this paper was to determine isothermal moisture profiles in a soil fill and predict the soil moisture movement above the ground water table through the use of explicit finite difference modeling. The methodology was successfully demonstrated through a real-world example. Although several numerical models are now available in the form of computer software to accomplish this, this paper is intended to demonstrate the steps involved in developing such computational models which would be greatly helpful for educators and students.

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