MILESTONE REPORT

Numerical Modeling of Preferential Flow at the Pantex Plant Area

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SUMMARY

The objective of this study was to analyze preferential flow on the basis of observations from four ponding tests conducted in the vicinity of the Pantex Plant. According to soil profiles exposed after the field ponding tests (Xiang et al., 1993), we derived the hydraulic conductivity of an equivalent homogeneous soil as that of the actual heterogeneous soil. Models of four different types of subsurface flow were considered. These include flow through the soil matrix, through root tubules, between ped faces, and along soil-filled cracks. The results of numerical simulations of matrix flow were similar to field observations of matrix flow from ponding tests. To evaluate preferential flow, different values of hydraulic conductivity were used. The simulations show that preferential flow results in an increased rate of water movement because of the higher equivalent hydraulic conductivity.

INTRODUCTION

Analysis of water flow through the unsaturated zone is important for estimation of ground-water recharge rates and for contaminant transport. Conventional numerical simulations ignore preferential flow, and the simulation results underestimate contaminant transport velocities in areas where preferential flow is important.

Singh et al. (1992) reviewed numerical models that can be applied to simulate contaminant transport in soils and concluded that deterministic models have provided valuable conceptual theories of transport mechanisms, although the applicability of these models to naturally variable field conditions has been questioned. They also pointed out that reliable field data that are used as input to the models may become the critical factor for determining the accuracy of these models. Dual-porosity models, which assume that a porous medium consists of two separate but connected continua, are often used. Gerke and van Genuchten (1993) developed a dual-porosity model for simulating preferential flow in structured porous media. They also reviewed papers that used the dual-porosity concept. McKay et al. (1993) provided a reliable determination of the magnitude and spatial distribution of hydraulically derived fracture parameters in a clay deposit. Previous studies of the effect of preferential flow on contaminant transport are limited (Richard and Steenhuis, 1988). Steenhuis et al.'s (1990) study indicated that preferential flow through worm borings and root channels in the surface layer may move contaminants directly to the ground water within a short time.

Four ponding tests conducted in the vicinity of the Pantex Plant indicate that preferential flow results in rapid downward movement of water (Xiang et al., 1993). If preferential flow is ignored, the results of numerical simulations will greatly underestimate the rate of water movement. To increase the accuracy of the simulations, preferential flow has to be considered.

The objective of this research was to develop mathematical models for preferential flow. Results of simulations that include preferential flow are compared with those of matrix flow.

MATHEMATICAL MODELS FOR OBSERVED PREFERENTIAL FLOW

Vertical Flow

Four ponding tests were conducted at TDCJ playa basin to track water flow along preferred pathways. Plots 1 and 2 were sited in grasslands on the eastern slope of the playa basin and Plots 3 and 4 were sited in the playa lake near its eastern edge. Water was dyed blue to record the spatial distribution of the preferential flow pathways. According to observations from four ponding test profiles (Xiang et al., 1993), water flow beneath the ponded surface can be expressed as

$$Q_z = Q_m + Q_r + Q_p + Q_c \tag{1}$$

where Q_z is the total flux through a cross sectional area A, Q_m is the flux through the soil matrix, Q_r is the flux through the gap between the roots and the surrounding soil, Q_p is the flux between ped faces, and Q_c is the flux through soil-filled cracks. In this model, the effect of horizontal flow is not considered because strong lateral flow was not observed from the ponding test profiles (Xiang et al., 1993). Animal burrows are also found in the study area and are much larger than the above pathways. However, because of the irregular distribution of these animal burrows, we did not consider their effects in the following models. According to Darcy's law, the flux is

$$Q_z = K_z(\theta)\frac{\partial h}{\partial z} \tag{2}$$

where h is the hydraulic head and z is the vertical coordinate. K_z is the equivalent hydraulic conductivity in the z direction, and it can be further written as

$$K_z = K_m + K_r + K_p + K_c \tag{3}$$

where K_m is the hydraulic conductivity of the soil matrix, K_r is the equivalent hydraulic conductivity of the space between roots and the surrounding soil, K_p is the equivalent hydraulic conductivity of ped faces, and K_c is the equivalent hydraulic conductivity of soil-filled cracks. Figure 1 illustrates the four elements, matrix flow (Fig. 1a), flow surrounding roots (Fig. 1b), flow between ped faces (Fig. 1c), and flow through soil-filled cracks (Fig. 1d). In the following, we present a mathematical model for each type of flow.

Matrix flow

Matrix flow is the basic type of flow considered in most models, and it is illustrated in Figure 1a. In this case, K_m is the hydraulic conductivity of the soil column without any fractures, roots, cracks, or ped faces. The value of K_m can be evaluated from water retention functions determined in the laboratory. Hydraulic conductivity is a function of water content. For a soil column with a cross sectional area A, flow can be expressed as

$$Q_m = K_m(\theta)\frac{\partial h}{\partial z}A \tag{4}$$

where the conductivity K_m can be determined from the following equation (Van Genuchten, 1980):

$$K_m(S_e) = K_s S_e [1-(1-S_e^{1/m})^m]^2 \tag{5}$$

where K_s is the saturated hydraulic conductivity of the soil matrix, and is the effective saturation and is defined as:

$$S_e = \frac{\theta - \theta_r}{\theta_s - \theta_r} \tag{6}$$

where θ is the water content, θ_s is the saturated water content, and θ_r is the residual water content. The effective saturation can also be expressed as a function of hydraulic head, i.e.,

$$S_e = \frac{1}{[1+(\alpha h)^n]^m} \tag{7}$$

where α, n, and m are parameters that can be determined from the retention curves.

Flow surrounding roots

Trenches dug after the ponding tests revealed that the surface soils contain a high density of grass roots. Tracer tests showed that roots are important channels for preferential flow, particularly in the interplaya area. Water flow along the gap between the root and the surrounding soil can be evaluated as water flow through a circular fracture. The flux through a capillary tube can be expressed by Poiseuille's law, i.e.,

$$Q = \frac{\pi r^4 \rho g}{8\mu} \frac{\partial h}{\partial l} \tag{8}$$

where r is the radius of a straight circular capillary tube, ρ is the fluid density, g is the gravitational acceleration, μ is the kinematic viscosity coefficient, and l is the coordinate along the fracture. The flow in the annular space between the soil and roots can be approximated by the difference between two tubes with radii r_r and r_p, respectively, where r_r is the radius of the root, and r_p is the radius of the hole in the soil surrounding the root. For an individual root, the flux through the gap can be written as

$$q_r = \frac{\pi\ (r_p^4 - r_r^4)}{8} \frac{\rho g}{\mu} \frac{\partial h}{\partial z} \qquad (9)$$

For a root tubule (most of them exist 2 to 3 m below the surface), $r_r = 0$ in equation (9). The total flow for m_r roots in an area A can be written as

$$Q_r = m_r \frac{\pi(\bar{r}_p^4 - \bar{r}_r^4)}{8} \frac{\rho g}{\mu} \frac{\partial h}{\partial z} \qquad (10)$$

where $\bar{r}_p$ is the average radius of the hole surrounding the roots and $\bar{r}_r$ is the average radius of roots. For root tubules, the hydraulic conductivity can be calculated by letting $\bar{r}_r = 0$ in equation (10).

Flow between ped faces

The water flow between ped faces can be treated as fissure flow if the conduit is idealized as the space between two parallel plates. It can be expressed as

$$q_p = \frac{b_p^3 \rho g}{12\mu} \frac{\partial h}{\partial z} l_p \qquad (11)$$

where q_p is the flow between the ped faces with b_p being the aperture and l_p being the length of the ped face. For m_p ped faces in the specified area A, the following equation may be used to calculate the total flow:

$$Q_p = m_p \frac{\bar{b}_p^3 \rho g}{12\mu} \frac{\partial h}{\partial z} \bar{l}_p \qquad (12)$$

where $\bar{b}_p$ is the average aperture of the ped face and $\bar{l}_p$ is the average length of the ped face.

Flow along soil-filled cracks

Filled cracks provide small channels for water flow compared with ped faces. If the porosity of the fill material is ϕ_c, then the flux along one filled crack may be expressed as

$$q_c = \frac{(\phi_c b_c)^3 \rho g}{12\mu} \frac{\partial h}{\partial z} l_c \qquad (13)$$

where b_c is the aperture of the filled crack. For m_c filled cracks, the total flux is

$$Q_c = m_c \frac{(\bar{\phi}_c \bar{b}_c)^3 \rho g}{12\mu} \frac{\partial h}{\partial z} \bar{l}_c \qquad (14)$$

where $\bar{\phi}_c$ is the average porosity of the fill material in the crack for a specified area A, $\bar{b}_c$ is the average aperture of filled cracks, and $\bar{l}_c$ is the average width of the filled crack. According to equations (1) and (2), we have the equivalent vertical conductivity

$$K_z(\theta) = \frac{Q_z}{\partial h / \partial x} \qquad (15)$$

Substituting (4), (10), (12), and (14) into (15), one has

$$K_z = K_m(\theta) + [m_r \pi(\bar{r}_p^4 - \bar{r}_r^4)/2 + m_p \bar{l}_p b_p^3 / 3 + m_c (\phi_c b_c)^3 \bar{l}_c / 3] \frac{\rho g}{4\mu A}] \qquad (16)$$

This is the equivalent vertical hydraulic conductivity, which reflects the effect of roots, ped faces, and soil-filled cracks on water infiltration in surficial soils. Using equation (15), the equivalent conductivity of root tubules is

$$K_r = m_r \pi(\bar{r}_p^4 - \bar{r}_r^4) \frac{\rho g}{8\mu A} \qquad (17)$$

the equivalent conductivity of ped faces is

$$K_p = m_p \bar{b}_p^3 \bar{l}_p \frac{\rho g}{12\mu A} \qquad (18)$$

and the equivalent conductivity of soil-filled cracks is

$$K_c = m_c (\bar{\phi}_c \bar{b}_c)^3 \bar{l}_c \frac{\rho g}{12\mu A} \qquad (19)$$

Once the vertical conductivity is determined, the subsurface flow can be simulated and the total flow rate should approximate the actual flow rate if estimates of the average root radius and root density, the average aperture, length, and density of ped faces and soil-filled cracks are appropriate.

SIMULATION OF WATER FLOW IN THE PANTEX PLANT AREA

Parameter estimation for the model

Hydraulic conductivity for matrix flow

Water-retention data were measured for three soil cores in the laboratory. These cores were collected from depths of 0.2 m, 0.4 m, and 0.6 m beside ponding test Plot 1 (Xiang et al., 1993). Retention curves were fitted to the data (Fig. 2). The saturated hydraulic conductivity was measured with a Guelph permeameter and the data analyzed according to the method developed by Xiang (1993). The measured saturated hydraulic conductivity is expected to be representative of the soil matrix between ped faces because root density was very low at the test location (0.8 m below the surface).

Geometric parameters

In order to determine the equivalent conductivity K_z, it is necessary to estimate the average number of roots, ped faces, and soil-filled cracks, as well as their spatial distribution in a specified area.

Roots

In the top part of the soil, the roots are very dense. Figure 3 presents the relationship of conductivity to the root radius based on equation (17) assuming that the hole surrounding the root has a radius of 0.3 mm, where m_r is the number of roots. This figure shows that when the gap between the soil and the roots is large, the conductivity increases. When m_r or the difference $r_p - r_r$ is large, the equivalent conductivity will increase greatly, and it is even higher for root tubules ($r_r = 0$). The average diameter of roots is about 0.5 mm, the soil hole has a diameter of about 0.6 mm (the largest root has a diameter of about 5 mm). Ignoring the very small root tubules (less than 0.1 mm), an estimate of root density is 4000 roots per m^2 for the top region. The length of roots varies from 0.2 to 1.0 m. The viscosity coefficient η is defined as the shear stress per unit shear rate and $\eta = \mu / \rho g$ (for water at 20 °C, $\eta = 1.0 \times 10^{-3}$ Pa·s). Based on this number, we can obtain an approximate equivalent conductivity.

Ped faces

We assume that the equivalent conductivity of ped faces equals that of an orthogonal network of vertical, equal-aperture, continuous fractures in the soil (as used by McKay et al., 1993), as shown in Figure 4. According to the profiles in ponding test Plot 1 (Xiang, 1993), the estimated interval between peds is 0.1 m in the 0 to 0.2 m depth zone and 0.4 m for the 0.2 to 1.0 m depth zone. The estimated average aperture of ped faces is 2 mm on the top, and it decreases with depth.

Soil-filled cracks

The density of soil-filled cracks is low and varies greatly. The estimated distance between these soil-filled cracks is 0.5 m. The average aperture of these soil-filled cracks is estimated as 4 mm, and it reduces to less than 1 mm below 1 m depth (data from cores show that the average aperture is less than 1 mm and the lateral spacing is about 0.1 m). The estimated average soil porosity in the cracks is 0.5. Based on these data, the equivalent conductivity can be obtained from equation (19).

Simulations

One-dimensional numerical simulations were conducted based on the following boundary conditions:

$$h = 0.1 \text{ m at } 0 < t < 0.125 \text{ day and } z = 0 \tag{20}$$

The infiltration rate is

$$q = 0.0 \text{ at } t > 0.125 \text{ day and } z = 0 \tag{21}$$

$$q = 0.0 \text{ at } t > 0 \text{ and } z = 1.0 \tag{22}$$

The initial water content was obtained from soil samples (silty clay) collected prior to ponding (Xiang et al., 1993) at every 0.2 m along a vertical profile. Only the top meter of the soil was simulated because this was the area evaluated in the ponding test and the other hydraulic parameters are also available from this area. Although we did not simulate water flow in deeper soil, the results may be similar, except that the preferential flow would be less because most fractures are closed and soil-filled cracks have smaller apertures. Two cases, matrix flow and preferential flow, are considered to demonstrate the differences between them.

Matrix flow

We used the computer code HYDRUS (Kool and van Genuchten, 1991) to perform the numerical simulations. Evaporation was not considered in the simulations. The boundary conditions are given by equations (20) through (22). To ensure convergence of the simulations, small time steps and small element sizes were used. Figure 5 illustrates the initial water content and water contents at different times as a function of depth based on simulations that used the parameters in Table 1. This figure illustrates that in the beginning, the water content in the upper portion increases greatly, then decreases, but the water content in the middle and bottom parts gradually increases. Figure 6 shows the matric potential as a function of depth. It illustrates that the bottom soil initially has low matric potential. With water infiltration, this low matric potential is gradually increased after several days.

Table 1. Fitted water retention parameters and the measured saturated conductivity by the Guelph permeameter test.

Location	θ_r	θ_s	α $(1/m)$	n	$m = 1-1/n$	l	K_s (m/s)
0.2	0	0.49285	0.1	1.1713	0.14625	0.5	4.83 E–7
0.4	0	0.5115	0.63	1.1078	0.09731	0.5	
0.6	0	0.5015	0.13	1.4095	0.29053	0.5	

The upper boundary condition in the above simulations was a constant head of 0.1 m. A series of simulations for different hydraulic heads were conducted. Figure 7 shows the water content as the function of depth for different hydraulic heads. It illustrates that the hydraulic head does not affect the matrix flow significantly.

Preferential flow

As we noted from the ponding tests, preferential flow is important in rapidly moving water in the subsurface. Because determination of geometric parameters related to preferential flow is highly uncertain, we evaluated the effect of preferential flow by calculating an equivalent hydraulic conductivity, as described previously. We used the proposed models for the different components of preferential flow such as roots, etc., and the same boundary conditions as were used for the matrix flow simulations. The results of the simulations are illustrated in Figure 8, where K_{ps} is the sum of the equivalent conductivities of roots, ped faces, and soil-filled cracks. This figure confirms that downward water movement increases as hydraulic conductivity increases as a result of preferential pathways.

The model developed here is only valid for a case involving the total flux; for contaminant transport, however, the arrival time is critical. In addition, variations in hydraulic head may strongly affect preferential flow.

CONCLUSIONS

Water flow through surficial sediments in the vicinity of the Pantex Plant can be divided into four elements: flow in the soil matrix, flow though root tubules, flow between ped faces, and flow along soil-filled cracks. Using Poiseuille's law for capillary tubes, we propose a model for flow through root tubules. To use this model, we need information on the average root size and the gap between the surrounding soil and the root, in the case of root tubules the radius of the tubule, and the root or root tubule density in a unit area. Water flow between ped faces and along soil-filled cracks can be approximated by the cubic law for parallel plates. The necessary information to determine the equivalent conductivity for these structures is the average size of the aperture, the length of the ped face or soil-filled crack, and the density of these structures in a unit area. We assume that the distribution of ped faces and soil-filled cracks can be approximated as an orthogonal network of vertical, equal-aperture, continuous structures in the soil.

Simulations for soil matrix flow show that water moves slowly downward. Variations in the ponding depth did not affect the rate and depth of water movement significantly. The effect of preferential flow was considered by calculating an equivalent hydraulic conductivity for the preferential flow structures, and the increased conductivity resulted in increased water fluxes.

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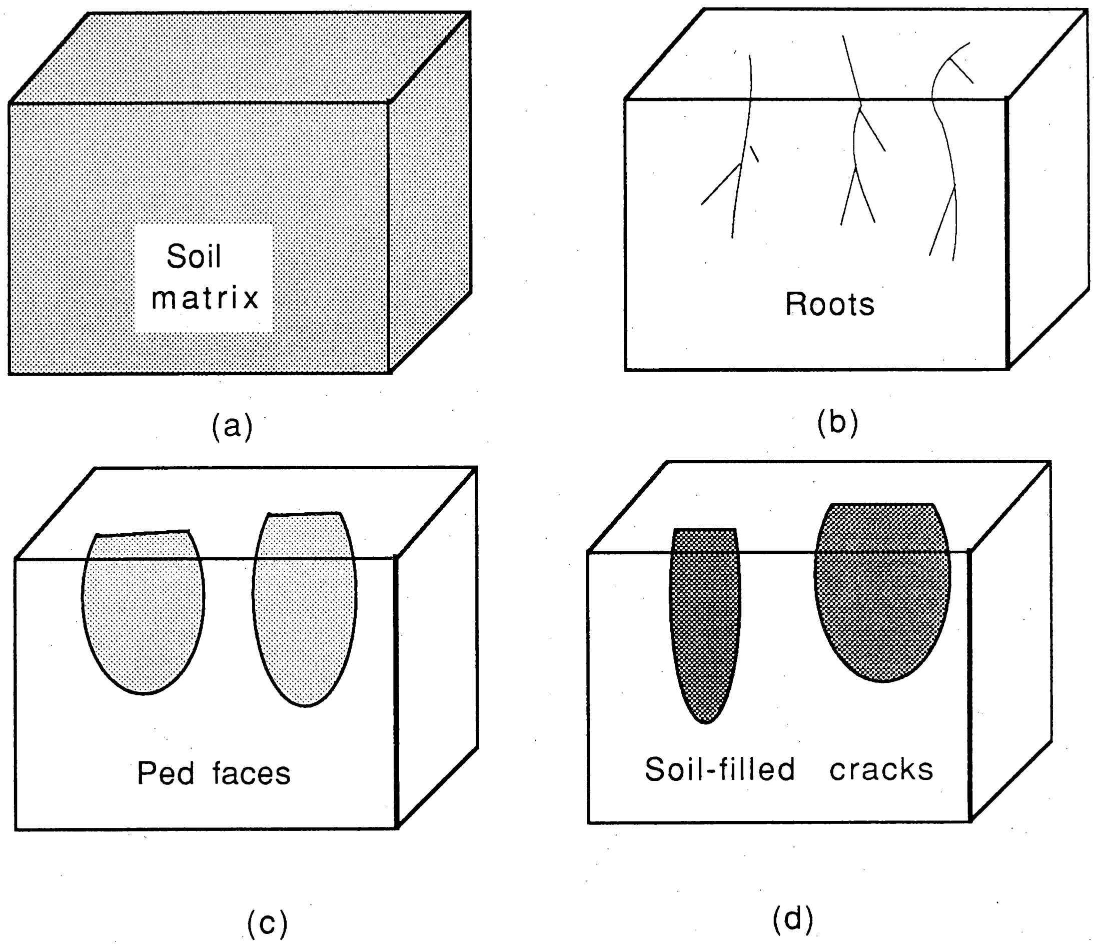

Figure 1. Models of water flow: (a) matrix flow, (b) flow surrounding roots, (c) flow between ped faces, and (d) flow through soil-filled cracks.

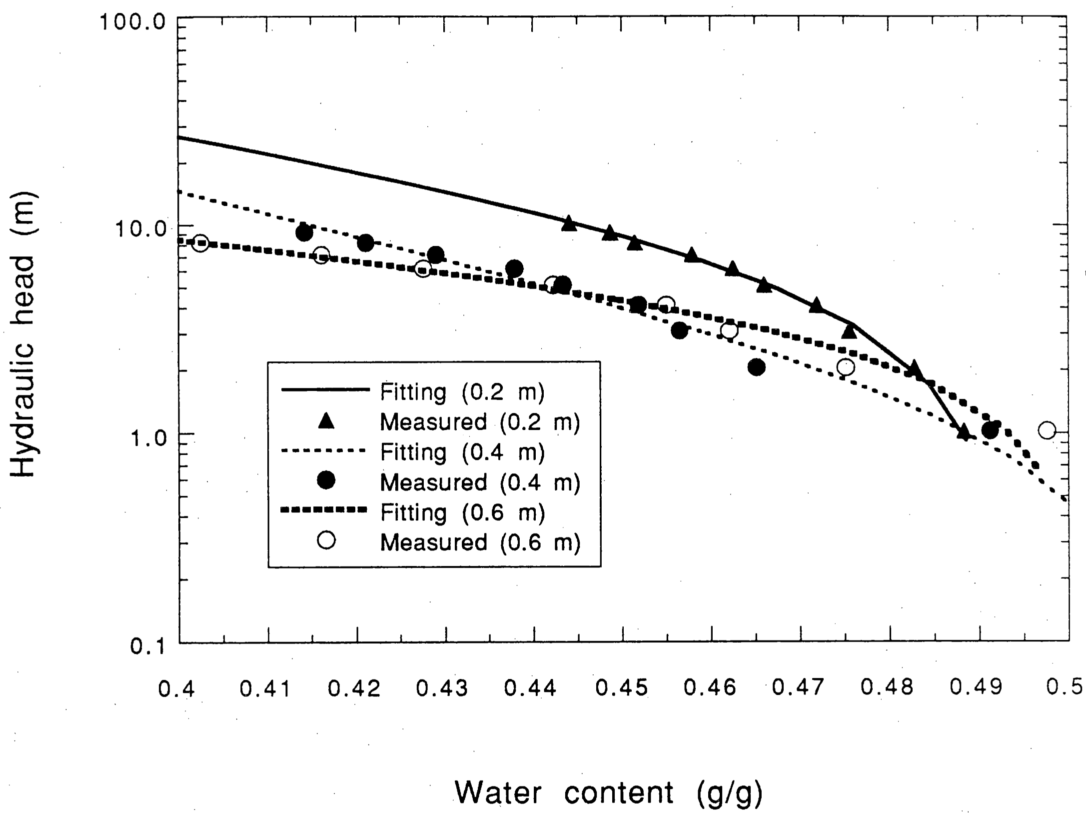

Figure 2. Retention data for soil samples at different locations.

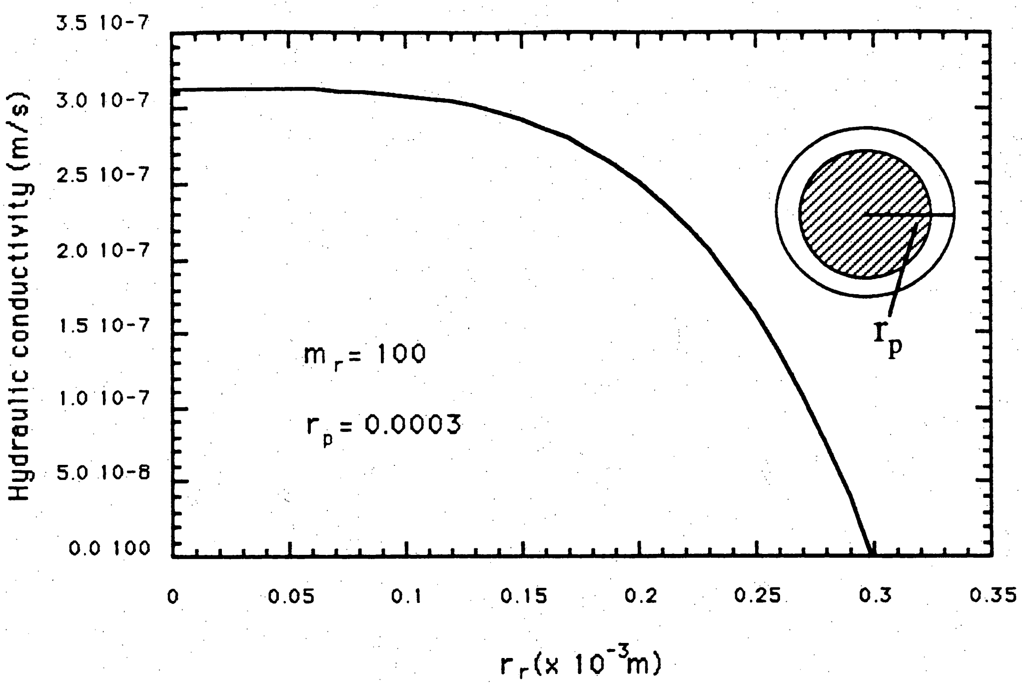

Figure 3. The relationship of hydraulic conductivity to root radius r_r (where we assume that the root tubule has a radius of 0.3 mm).

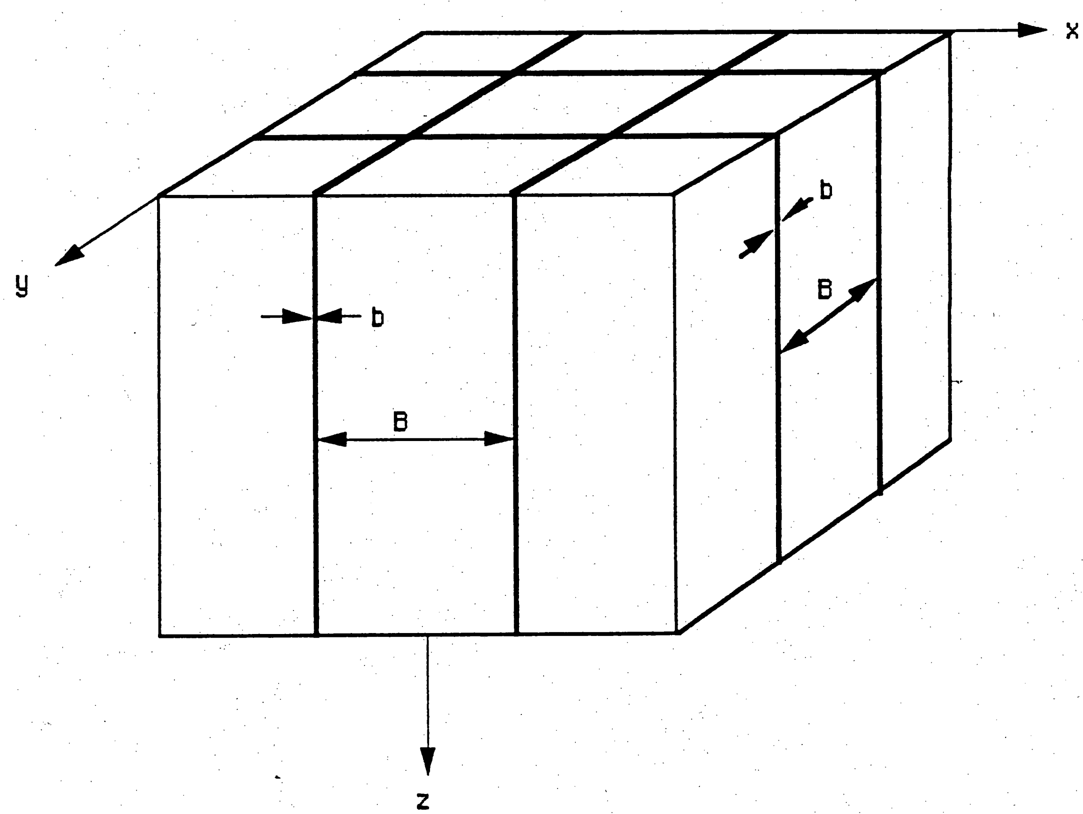

Figure 4. An idealized ped face and crack model, where b is the aperture and B is the interval between ped faces.

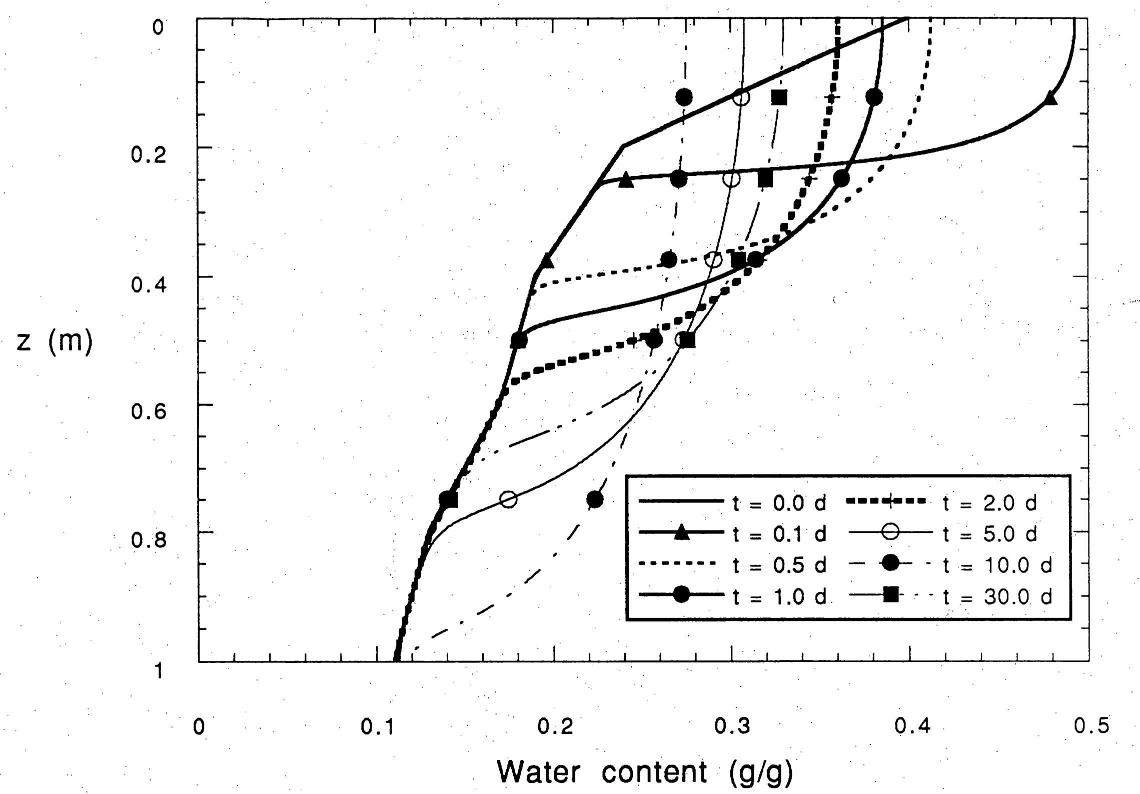

Figure 5. The simulated water content at different times and depths.

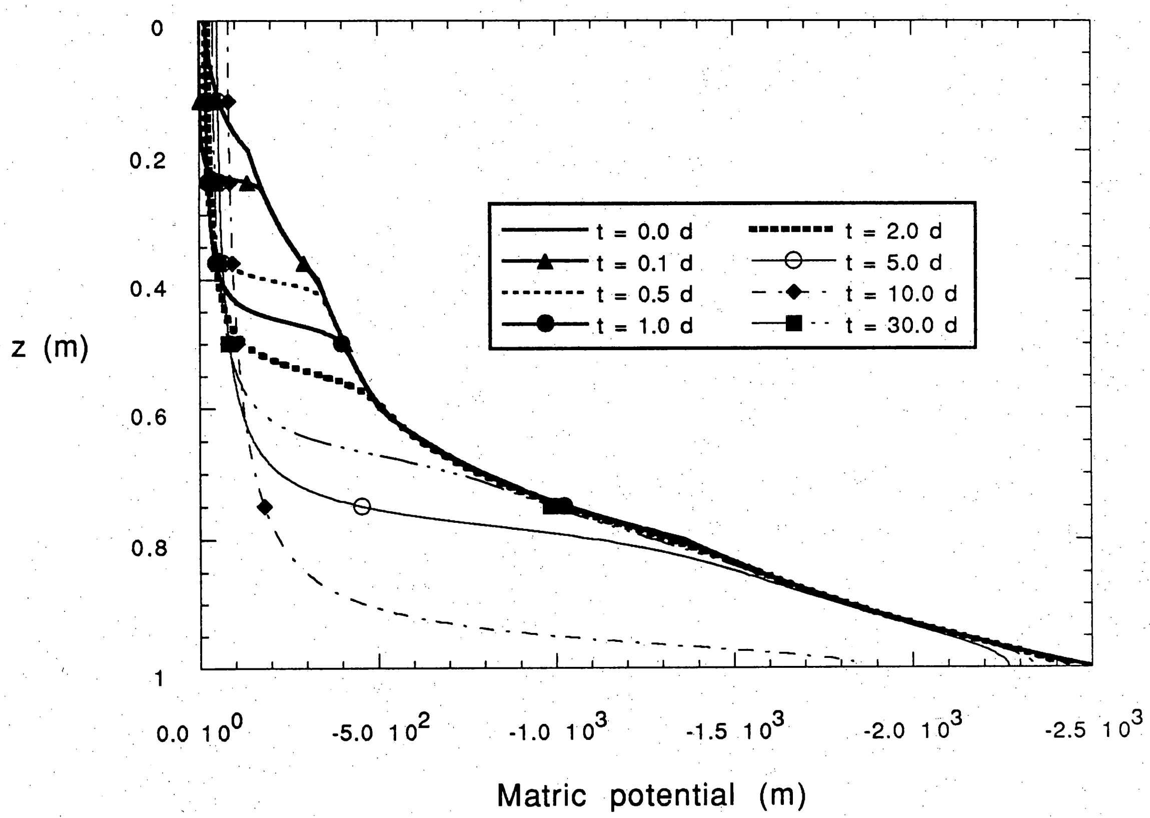

Figure 6. The simulated matric potential at different times and depths.

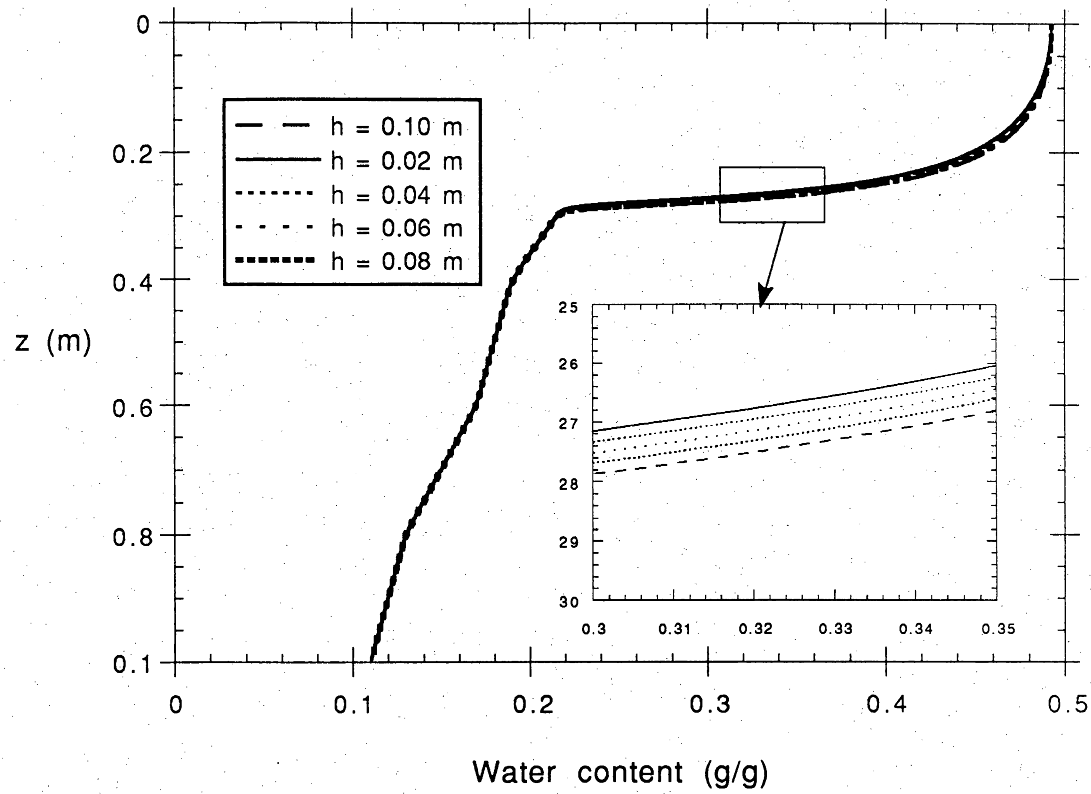

Figure 7. The simulated water content at 0.1 day for different hydraulic heads, where the hydraulic head is constant from time 0 to 0.125 day.

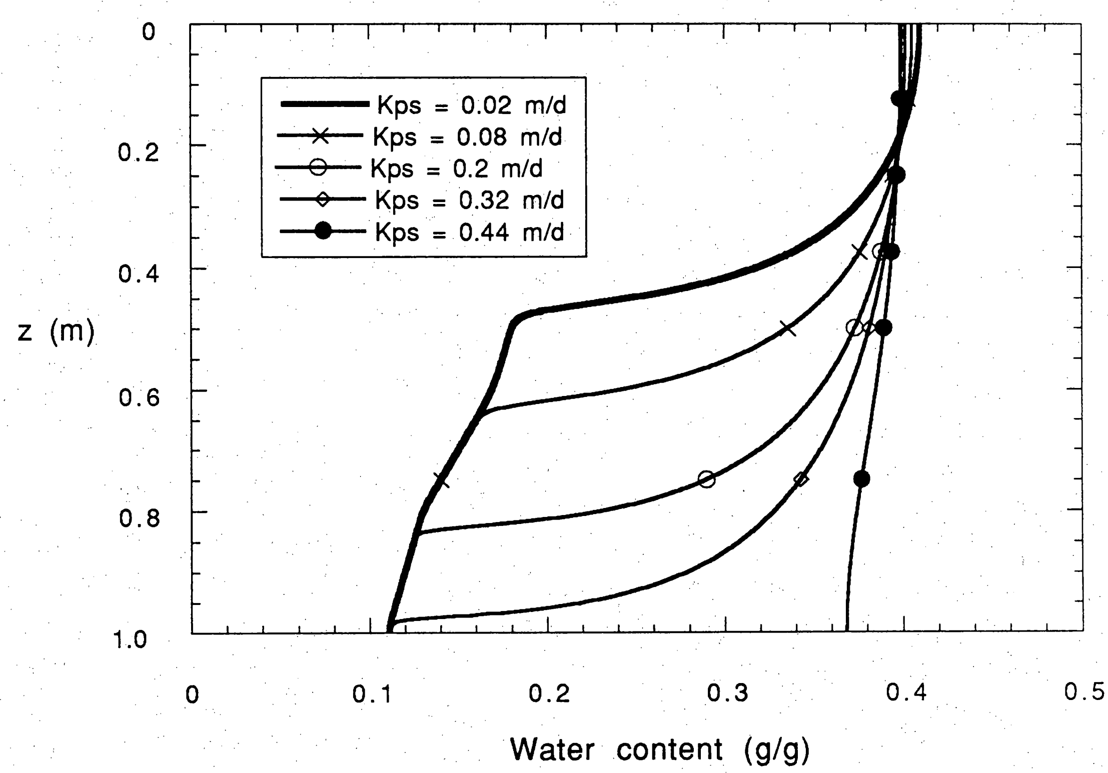

Figure 8. The simulated water content for different values of K_{ps} (where K_{ps} is the sum of the equivalent conductivity of root tubules, ped faces, and soil-filled cracks).