

Modeling flow and transport processes at the local scale

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Abstract. Much progress has been made during the past several decades in attempts to more realistically simulate variably-saturated water flow and solute transport in the subsurface. A large number of conceptual models are now available to predict flow and transport in the vadose zone. In this paper we highlight recent advances in modeling at especially the local scale. Improved understanding of underlying processes, continued advances in numerical methods, and the introduction of increasingly powerful computers now permit comprehensive simulations of the most important physical, chemical and biological processes operative in the unsaturated zone. Examples include models for mass/energy transport in the soil-plant atmosphere continuum, multicomponent major ion chemistry, and multifluid flow. While the problem of preferential flow remains a challenge, several useful approaches have recently become available to study and model preferential flow in structured media. Increasingly accurate indirect methods, including pedotransfer functions, are now also available for estimating the unsaturated soil hydraulic properties from more readily available or easily measured data. A need still exists for more user-friendly software to enable more effective application of models to a variety of flow and transport problems in research and management.

Introduction

As measured against the many hundreds of thousands of years of human life on earth, and the several thousands of years of cultivating the earth's surface and practicing irrigation, we have only very recently begun to unravel in a systematic fashion the fundamental processes affecting water and solute movement in the unsaturated (vadose) zone between the soil surface and the groundwater table. Progress is indeed tremendous if one realizes that Darcy's law for saturated flow was first proposed only some 150 years ago (Darcy, 1856), while the Richards equation for unsaturated flow was first formulated less than 70 years ago (Richards, 1931). Advances in process-based understanding of subsurface flow and transport, numerical analysis and computer hardware during especially the last 30 years or so have been truly astonishing. Now, for the first time, opportunities exist to couple into a unified quantitative numerical approach the many factors influencing water and solute movement in the subsurface. Unfortunately, while much progress has been made, so has the urgency by which solutions are needed; this in view of increasing soil and water pollution problems in a world with limited soil and water resources.

In this paper we summarize recent progress in variably-saturated flow and transport modeling at especially the local scale. Topics to be addressed include traditional approaches for modeling flow and transport, plant-root water uptake, multicomponent chemical transport, preferential flow, and methods for estimating the unsaturated soil hydraulic properties. Parts of this paper are adapted from two previous reviews (van Genuchten et al., 1997; van Genuchten & Sudicky, 1999). No attempt is made to cover all aspects related to water and solute transport in the subsurface.

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Governing equations for water, heat and solute movement

Predictions of water, heat and solute movement in the vadose zone are traditionally made using the Richards equation for variably-saturated water flow and advection-dispersion type equations for heat and solute movement. For a one-dimensional soil profile these equations are given by (e.g., Simunek et al., 1996)

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

$$\frac{\partial C_p(\theta)T}{\partial t} = \frac{\partial}{\partial z} \left[\lambda(\theta) \frac{\partial T}{\partial z} \right] - C_w \frac{\partial qT}{\partial z} - C_w ST \quad (2)$$

$$\frac{\partial(\rho s)}{\partial t} + \frac{\partial(\theta c)}{\partial t} = \frac{\partial}{\partial z} \left(\theta D \frac{\partial c}{\partial z} - qc \right) - \phi \quad (3)$$

respectively, where θ is the volumetric water content, h is the soil water pressure head, t is time, z is distance from the soil surface downward, K is the hydraulic conductivity as a function of h or θ , λ is the apparent thermal conductivity of the soil, C_p and C_w are volumetric heat capacities of the porous medium and the liquid phase, respectively; T is temperature, s is the solute concentration associated with the solid phase of the soil, c is the solute concentration of the liquid phase, ρ is the soil bulk density, D is the solute dispersion coefficient, q is the volumetric fluid flux density given by Darcy's law, and S and ϕ are sinks or sources for water and solutes, respectively;. Similar equations may be formulated for multi-dimensional flow and transport.

Models based on Eqs. (1), (2) and (3) have proved to be important tools in research and management. Still, the equations are based on a large number of simplifying assumptions, which limit their applicability (Nielsen et al., 1986). The equations assume that (a) the air phase plays a relatively minor role during unsaturated flow, and hence that a single equation can be used to describe variably-saturated flow, (b) Darcy's equation is valid at both very low and very high flow velocities (including those occurring in structured soils), (c) the osmotic and electrochemical gradients in the soil water potential are negligible, (d) the fluid density is independent of the solute concentration, and (e) matrix and fluid compressibilities are relatively small. The equations are further complicated by the hysteretic nature of especially the soil water retention function, $\theta(h)$, the extreme nonlinearity of the hydraulic conductivity function, $K(h)$, the lack of accurate and inexpensive methods for measuring the unsaturated hydraulic properties, the effects of temperature and soil solution chemistry on the unsaturated soil hydraulic properties, and inconsistencies between the scale at which the flow and transport parameters in Eqs. (1) to (3) are usually measured, and the scale at which the models are being applied.

Root water uptake

The source/sink term S in Eq. (1) accounts for water uptake by plant roots. This term is critical in terms of predicting water and solute dynamics in the soil root zone, and for simulating transpiration and crop growth. Many of the early studies of root water uptake used uptake functions of the general form (e.g., Bresler et al., 1982)

$$S(z,t) = -b(z)K(\theta)[h_r - h(z,t) - \pi(z,t)] \quad (4)$$

where h_r is an effective root-water pressure head, π is the osmotic head, and b a depth-dependent proportionality constant often referred to as the root effectiveness function. Equation (4) may be viewed as a finite difference approximation of Darcy's law across the soil-root interface. Another class of root-water uptake models, used in our research, is given by (Simunek & Suarez, 1993)

$$S(z,t) = \beta(z) \alpha_s(h) \alpha_\pi(\pi) T_p \quad (5)$$

where $\beta(z)$ is the potential root water uptake distribution function which integrates to unity over the soil root zone, α_s and α_π are dimensionless water and salinity stress response functions between 0 and 1, and T_p is the potential transpiration rate. Cardon & Letey (1992), among others, showed that Eq. (5) may be preferred as compared to extraction functions given by Eq. (4). Equation (4) was found to lead to unrealistic shifts between optimal and zero transpiration as compared to experimental data. The equation also failed to predict significant decreases in transpiration under highly saline conditions.

The water and salinity stress response functions, $\alpha_s(h)$ and $\alpha_\pi(h)$, in (5) are prescribed dimensionless functions of the soil water pressure head and osmotic head (van Genuchten, 1987; van Genuchten & Gupta, 1993) as follows

$$\alpha_s(h) = \frac{1}{1 + (h/h_{50})^{b_1}} \quad \alpha_\pi = \frac{1}{1 + (\pi/\pi_{50})^{b_2}} \quad (6a,b)$$

where h_{50} , π_{50} , b_1 and b_2 are empirical constants. The parameters h_{50} and π_{50} represent the pressure and osmotic heads where the water extraction rate is reduced by 50% due to either water or salinity stress. Equation (6a) for $\alpha_s(h)$, in contrast to an earlier approach by Feddes et al. (1978), does not consider a reduction in transpiration at pressure heads near saturation. The decrease in uptake sometimes observed near saturation is related to oxygen stress and may be more properly treated using predictions of the gas phase composition, provided a suitable model is used to account for CO₂ production and transport (Suarez & Simunek, 1993). An alternative to Eq. (6b) is the traditional threshold-slope salt-tolerance response model (Maas & Hoffman, 1977).

The normalized potential water uptake rate function, $\beta(z)$, describes the spatial variation of the potential uptake rate over the root zone. Many expressions have been used for $\beta(z)$, including equations that are constant with depth, linear, exponential with a maximum at the soil surface, or a trapezoidal function (van Genuchten & Hoffman, 1983). The actual transpiration rate, T_a , is obtained by integrating the root water uptake rate over the root zone as follows

$$T_a = \int_0^{L_r} S(h,\pi,z) dz = T_p \int_0^{L_r} \alpha_s(h) \alpha_\pi(\pi) \beta(z) dz \quad (7)$$

where L_r is the rooting depth, can be made either constant or variable during a simulation. For annual crops or certain long-term simulations a growth model may be required to account for changes in L_r with time (e.g., Simunek et al., 1996).

Multicomponent chemical transport

Equation (3) describes the transport of a single ionic species in the presence or absence ($s=0$) of solute sorption by the soil solid phase. The approach ignores the fact that the soil liquid phase always contains a mixture of many ions that may interact, create complex species, precipitate, dissolve, and/or compete with each other (especially the cations Na, Ca and K) for sorption sites on the solid phase. These processes become dominant in many salt-affected soil systems, especially during reclamation of sodic soils. Hence, accurate simulation of transport in salt-affected soils requires the use of multicomponent transport models. Here we briefly summarize the UNSATCHEM models (Simunek & Suarez, 1993, 1994; Simunek et al., 1996) that consider multicomponent transport. The models account for major ion chemistry, multiphase gas transport, CO₂ production/transport and heat transport. Soil temperature is required for predicting CO₂ production, as well as for evaluating thermodynamic equilibrium and kinetic rate constants. The CO₂ concentration in turn is needed to predict pH and the soil solution composition.

One-dimensional multicomponent transport during transient variably-saturated flow may be described with the equations (Simunek & Suarez, 1994)

$$\frac{\partial(\theta c_k)}{\partial t} + \rho \frac{\partial \bar{c}_k}{\partial t} + \rho \frac{\partial \hat{c}_k}{\partial t} = \frac{\partial}{\partial z} \left(\theta D \frac{\partial c_k}{\partial z} - q c_k \right) \quad k = 1, 2, \dots, n_s \quad (8)$$

where c_k , \bar{c}_k and \hat{c}_k are the total dissolved, sorbed and mineral (precipitated) concentrations, respectively, of aqueous component k , and n_s is the number of aqueous components. The second and third terms on the left-hand side of (8) are zero for components that do not undergo ion exchange and precipitation/dissolution reactions. The total concentration of a component k , defined as the sum of the dissolved, sorbed and mineral concentrations, is influenced only by transport processes which act on the solution concentration c_k , but not by chemical reactions. However, the relative fraction of a component in each of the three phases (solution, sorbed, mineral) depends strongly on the specific chemical processes in the system. Therefore, (8) must be augmented with equations describing the different equilibrium and nonequilibrium chemical reactions such as complexation, cation exchange, and precipitation/dissolution.

The chemical submodel in UNSATCHEM is a speciation program that considers cation exchange using Gapon type expressions, and has provisions for either equilibrium partitioning with solid phases or dissolution-precipitation reactions using kinetic expressions. A total of 33 chemical species (Table 1) were considered for a recent application to sodic soil reclamation (Simunek & Suarez, 1997). The model considered precipitation of gypsum, calcite, sepiolite, hydromagnesite, and nesquehonite whenever the calculated solution composition exceeded saturation for these phases. If any of these phases is specified as being present in the soil, the model can force the solution to go to saturation. The model assumed that the cation exchange capacity, CEC, is constant and independent of pH .

Precipitation-dissolution of calcite may be modeled using either equilibrium or kinetic expressions, while dissolution of dolomite is always treated as a kinetic process (Simunek & Suarez, 1994). The precipitation-dissolution of equilibrium solids is expressed in terms of solubility products K_{sp} . The species in the last group of Table 1 are represented by Henry's Law, the first and second dissociation equation for carbonic acid, the dissociation equation for water, and the charge balance equation. The entire system of equations is closed by electric charge balance equation, which allows calculation of pH .

Table 1. Species considered in the chemical submodel of UNSATCHEM (Simunek & Suarez, 1997)

1	Aqueous components	7	Ca^{2+} , Mg^{2+} , Na^+ , K^+ , SO_4^{2-} , Cl^- , NO_3^-
2	Complexed species	10	CaCO_3^0 , CaHCO_3^+ , CaSO_4^0 , MgCO_3^0 , MgHCO_3^+ , MgSO_4^0 , NaCO_3^- , NaHCO_3^0 , NaSO_4^- , KSO_4^-
3	Precipitated species	5	CaCO_3 , $\text{CaSO}_4 \cdot 2\text{H}_2\text{O}$, $\text{MgCO}_3 \cdot 3\text{H}_2\text{O}$, $\text{Mg}_5(\text{CO}_3)_4(\text{OH})_2 \cdot 4\text{H}_2\text{O}$, $\text{CaMg}(\text{CO}_3)_2$
4	Sorbed species	4	$\bar{\text{Ca}}$, $\bar{\text{Mg}}$, $\bar{\text{Na}}$, $\bar{\text{K}}$
5	CO_2 - H_2O species	7	P_{CO_2} , H_2CO_3^* , CO_3^{2-} , HCO_3^- , H^+ , OH^- , H_2O

Numerous methods have previously been proposed and used for reclaiming sodic soils, including the application of gypsum to the soil surface or in the irrigation water, incorporation of gypsum into the upper soil profile, adding acid to calcareous soil, leaching calcareous soils with high quality water, and incorporating acidic organic matter or waste products into the soil to reduce pH and enhance CO_2 production and dissolution of calcite (Simunek & Suarez, 1997). The UNSATCHEM models provide important tools for evaluating such methods for site-specific conditions. Using the one-dimensional version, Simunek & Suarez (1997) showed the importance of CO_2 dynamics in controlling the effectiveness of the different reclamation methods. For example, flooding combined with CO_2 production was found to elevate CO_2 concentrations in the root zone, resulting in a relatively effective reclamation practice. Application of acid water to calcareous soil with elevated CO_2 concentrations was shown to be the most effective. These findings are in general agreement with field data. Also, incorporating gypsum into the soil profile was found to be more effective than application of gypsum-saturated water.

Preferential flow

One major frustrating issue facing soil scientists and hydrologists in dealing with the unsaturated zone, both in terms of modeling and experimentation, is the overwhelming heterogeneity of the subsurface. One manifestation of heterogeneity at the local scale involves the preferential movement of water and chemicals through soil macropores or rock fractures. Preferential flow is caused by a broad array of processes and porous media properties. In unsaturated fractured rock water may move preferentially through fractures and fissures, while bypassing much of the rock matrix. The same process occurs in structured or macroporous soils where water may move through interaggregate pores, decayed root channels, earthworm burrows, and drying cracks in fine-textured soils. The term macropore flow is often used to describe the bypassing (short-circuiting) process in structured soils. A major difference between preferential flow in fractured rock vs. that in soils is the fact that near-surface processes in soils, such as shrink-swell, freeze-thaw, biological activity (leading to earthworm holes and root channels) and physical manipulation (e.g., cultivation of agricultural fields), can dynamically alter the preferential flow pathways, thus leading to temporal variations in the preferential flow process. Such temporal variations tend to decrease with depth where fractured rock often also dominates.

Preferential flow may also occur in seemingly homogeneous (especially coarse-textured) soils in the form of unstable flow (often called fingering) induced by soil textural layering, water repellency and air entrapment (e.g., Ritsema et al., 1993; Wang et al., 1998). In addition, preferential flow may be caused by funneling of water through high-conductivity layers, or as being redirected by sloping less-permeable layers. Often several of the above processes causing preferential flow to act together and/or reinforce each other. An important implication of

preferential flow is the accelerated movement of surface-applied fertilizers, pesticides, non-aqueous phase liquids, or other pollutants, into and through the unsaturated zone.

Process-based descriptions of preferential flow in structured media invoke dual-porosity or dual-permeability models. Such models typically assume that the medium consists of two interacting pore regions, one associated with the macropore or fracture network, and one with the micropores inside soil aggregates or rock matrix blocks. Different formulations arise depending upon how water and solute movement in the micropore region are modeled, and how water and solutes between the micropore and macropore regions are allowed to interact. Early formulations in the soil science and hydrology literature generally assumed the presence of distinct mobile and immobile (non-moving) liquid flow regions. Several studies have extended these models to variably-saturated flow conditions. Below we briefly review both steady-state and variably-saturated flow models applicable to structured media.

Models applicable to steady-state flow

A rigorous analysis of solute transport in structured soils can be made when the medium is assumed to contain geometrically well-defined cylindrical, rectangular or other types of macropores or fractures. Models may be formulated by assuming that the chemical is transported by advection, and possibly by diffusion and dispersion, through the macropores, while diffusion-type equations are used to describe the transfer of solutes from the larger pores into the micropores of the soil matrix. As an example, the governing equations for transport through media containing parallel rectangular voids are given by (e.g., van Genuchten & Dalton, 1986)

$$\mathcal{G}_f R_f \frac{\partial c_f}{\partial t} + \mathcal{G}_m R_m \frac{\partial c_m}{\partial t} = \mathcal{G}_f D_f \frac{\partial^2 c_f}{\partial z^2} - \mathcal{G}_f v_f \frac{\partial c_f}{\partial z} \quad (9)$$

$$R_m \frac{\partial c_a}{\partial t} = D_a \frac{\partial^2 c_a}{\partial x^2} \quad (-a \leq x \leq a) \quad (10)$$

$$c_m(z, t) = \frac{1}{a} \int_0^a c_a(z, x, t) dx \quad (11)$$

where the subscripts f and m refer to the interaggregate (fracture f) and intra-aggregate (matrix m) pore regions, respectively, $c_a(z, x, t)$ is the local concentration in the aggregate, x is the horizontal coordinate, z the vertical coordinate, and D_a the effective soil or rock matrix diffusion coefficient. Equation (9) describes vertical transport through the fractures, while (10) accounts for linear diffusion in a slab of width $2a$ in the horizontal (x) direction. Equation (11) represents the average concentration of the immobile soil matrix liquid phase. Equations (8) and (9) are coupled using the assumption of concentration continuity across the fracture/matrix interface:

$$c_a(z, a, t) = c_f(z, t) \quad (12)$$

The water contents \mathcal{G}_f and \mathcal{G}_m in (9) are given in terms of the bulk soil volume, i.e.,

$$\mathcal{G}_f = w_f \theta_f \quad \mathcal{G}_m = (1 - w_f) \theta_m \quad (13)$$

where w_f is the volume of the fractures relative to that of the total soil pore system. The total water content (θ) of the fracture/matrix system is given by the sum of \mathcal{G}_f and \mathcal{G}_m (using this formulation $\theta_f=1$ for a fully saturated fracture). Similar models as above may be formulated for other aggregate or soil matrix geometries (van Genuchten, 1985; van Genuchten & Dalton, 1986).

Geometry-based transport models have been successfully applied to laboratory-scale experiments as well as to selected field studies involving mostly saturated conditions. While geometry-based models are conceptually attractive, they may be too complicated for routine applications since structured soils and rocks usually contain a mixture of aggregates of various sizes and shapes. The problem of macropore and fluid flow continuity is also not easily addressed with geometry-based flow models. The issue of fluid flow continuity may be especially critical in the vadose zone because of possible preferential flow and channeling within the fracture domain itself during unsaturated conditions. Moreover, preferential flow paths may well change with the degree of saturation during unsaturated flow.

Rather than using geometry-based transport models, many of the preferential flow features can also be accounted for by using dual-porosity type models which assume simple first-order exchange of solutes by diffusion between the macropore (mobile) and micropore (immobile) liquid regions. The governing equations become then

$$\mathcal{G}_f R_f \frac{\partial c_f}{\partial t} + \mathcal{G}_m R_m \frac{\partial c_m}{\partial t} = \mathcal{G}_f D_f \frac{\partial^2 c_f}{\partial z^2} - \mathcal{G}_f v_f \frac{\partial c_f}{\partial z} \quad (14)$$

$$\mathcal{G}_m R_m \frac{\partial c_m}{\partial t} = \alpha (c_f - c_m) \quad (15)$$

where α is a first-order solute mass transfer coefficient characterizing diffusional exchange of solutes between the mobile and immobile liquid phases. Notice that (14) is identical to (9) for the rectangular geometry-based model. The mass transfer coefficient is of the general form

$$\alpha = \frac{\beta \mathcal{G}_m D_a}{a^2} \quad \alpha = \frac{\beta \mathcal{G}_m D_a}{(\xi_0 - 1)^2} \quad (16a,b)$$

where β is a geometry-dependent shape factor, and a is the characteristic length of the aggregate (e.g., the radius of a spherical or solid cylindrical aggregate, or half the width of a rectangular aggregate). Equation (16b) holds for a hollow cylindrical macropore for which $\xi_0 = b/a$ where a now represents the radius of the macropore and b the outer radius of the cylindrical soil mantle surrounding the macropore. The value of β ranges from 3 for rectangular slabs to 15 for spherical aggregates (Bolt, 1979; van Genuchten & Dalton 1986).

Extension to transient, variably-saturated flow

Different types of models have been proposed to extent the above dual-porosity approach to variably-saturated structured media. Here we summarize the dual-permeability model developed by Gerke & van Genuchten (1993, 1996). This model assumes that the Richards equation for transient water flow and the advection-dispersion equation for solute transport can be applied to each of the two pore systems. Similar to the first-order mobile-immobile approach (Eqs. 14 and 15), water and solute mass transfer between the two pore systems is described with first-order rate equations. The flow equations for the fracture (subscript f) and matrix (subscript m) pore

systems are, respectively,

$$C_f \frac{\partial h_f}{\partial t} = \frac{\partial}{\partial z} (K_f \frac{\partial h_f}{\partial z} - K_f) - \frac{\Gamma_w}{w_f} \quad (17)$$

$$C_m \frac{\partial h_m}{\partial t} = \frac{\partial}{\partial z} (K_m \frac{\partial h_m}{\partial z} - K_m) + \frac{\Gamma_w}{1-w_f} \quad (18)$$

where Γ_w describes the rate of exchange of water between the fracture and matrix regions:

$$\Gamma_w = \alpha_w (h_f - h_m) \quad (19)$$

in which α_w is a first-order mass transfer coefficient for water:

$$\alpha_w = \frac{\beta}{a^2} K_a \gamma_w \quad (20)$$

where β and a are the same as before, K_a is the hydraulic conductivity of the fracture/matrix interface, and γ_w (=0.4) is a dimensionless scaling factor. Solute transport in the fracture and matrix domains are described by, respectively:

$$\frac{\partial}{\partial t} (\theta_f R_f c_f) = \frac{\partial}{\partial z} (\theta_f D_f \frac{\partial c_f}{\partial z} - q_f c_f) - \frac{\Gamma_s}{w_f} \quad (21)$$

$$\frac{\partial}{\partial t} (\theta_m R_m c_m) = \frac{\partial}{\partial z} (\theta_m D_m \frac{\partial c_m}{\partial z} - q_m c_m) + \frac{\Gamma_s}{1-w_f} \quad (22)$$

where Γ_s is the solute mass transfer term given by

$$\Gamma_s = \alpha (c_f - c_m) + \begin{cases} \Gamma_w \vartheta_f c_f / \theta & \Gamma_w \geq 0 \\ \Gamma_w \vartheta_m c_m / \theta & \Gamma_w < 0 \end{cases} \quad (23)$$

in which α is the same as used in the first-order mobile-immobile model. The first term on the right-hand side of (23) specifies the diffusion contribution to Γ_s , and the second term the advective contribution. The above dual-permeability transport model reduces to the first-order model for conditions of steady-state flow in the fracture (macropore) region and no flow in the matrix pore system ($q_m = \Gamma_w = 0$).

The dual-permeability model given by Eqs. (17) through (23) contains two water retention functions, one for the matrix and one for the fracture pore system, but three hydraulic conductivities functions: $K_f(h_f)$ for the fracture network, $K_m(h_m)$ for the matrix, and $K_a(h)$ for the fracture/matrix interface. Of these functions, $K_f(h_f)$ is determined primarily by the structure of the fracture pore system, i.e., the size, geometry, continuity and wall roughness of the fractures, and possibly the presence of fracture fillings. Similarly, $K_m(h_m)$ is determined by the hydraulic

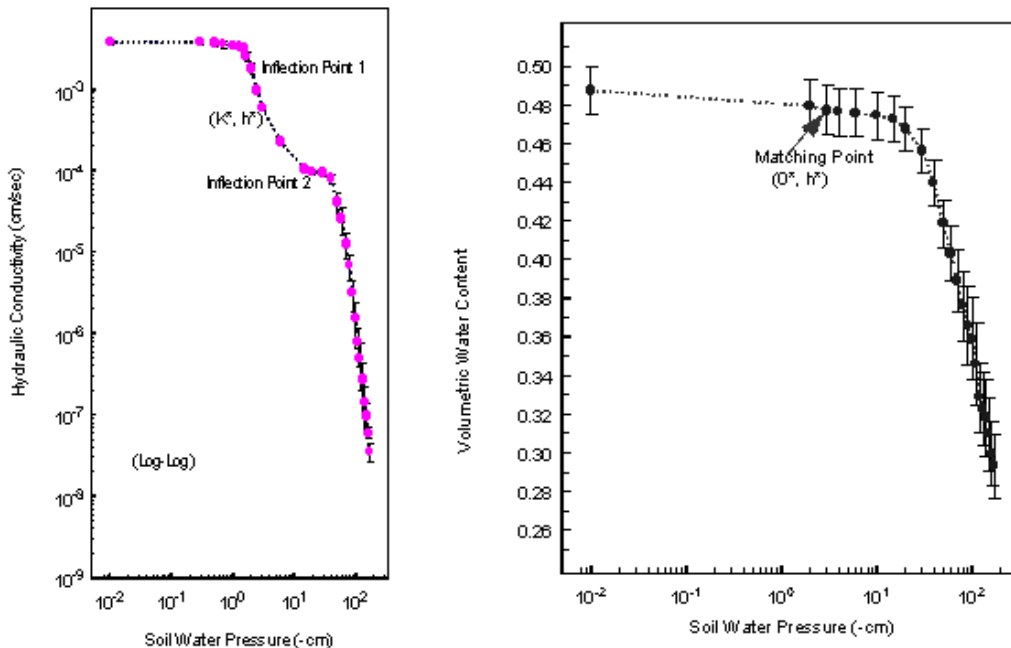


Figure 1. Plots of the field-averaged hydraulic conductivity function (geometric means and standard errors, left) and the field-averaged soil water retention function (arithmetic means and standard errors) for the surface horizon at the Las Nutrias experimental site (after Mohanty et al., 1997).

properties of single matrix blocks, and the degree of hydraulic contact between adjoining matrix blocks during unsaturated flow. Finally, $K_a(h)$ is the effective hydraulic conductivity function to be used in Eq. (20) for describing the exchange of water between the two pore systems. Estimates for the K_f - and K_m -functions may be obtained by assuming that K_f is primarily the conductivity function in the wet range, while K_m is the conductivity in the dry range (Peters & Klavetter, 1988; Durner, 1994).

Measurements of the composite (fracture plus matrix) hydraulic properties are greatly facilitated by the use of disc infiltrometers. Disc infiltrometry methods involving ponded and tension infiltrometers are now increasingly used for in situ measurements of the hydraulic conductivity at low soil water tensions. Advantages of these methods are that negative soil water pressures at the soil-infiltrator interface can be maintained very close to zero, and that they can be decreased in small increments to yield well-defined conductivity functions near saturation. Figure 1 shows field-averaged composite hydraulic functions for a macroporous site in New Mexico (Mohanty et al., 1997) obtained with ponded and tension infiltrometer measurements following experimental procedures as described by Ankeny (1992), and more standard laboratory $K(h)$ measurements on 5-cm long soil cores at higher suctions. The hydraulic conductivity data obtained with the ponded infiltrometer, tension infiltrometer, and laboratory experiments are superimposed across the tension range from 0 to 1.7 m for all measurement sites. Notice from Figures 1a and 1b that the hydraulic conductivity changes about 10 times or more in the near-saturated region (between saturation and 10 cm tension), while water retention changes only very little.

In several studies (Zurhhl & Durner, 1996; Mallants et al., 1996; Durner, 1994; Othmer et al., 1991), the hydraulic properties of bimodal or multimodal soils have been modeled using sums of several van Genuchten-Mualem type functions. The same is true for flow in unsaturated

fractured rock (e.g., Peters & Klavetter, 1988). Others (Jarvis & Messing, 1995; Wilson et al., 1992) used for this purpose a number of piecewise-continuous Russo-Gardner (Russo, 1988) type functions, joined at different junction points. To describe the data in Figure 1 accurately, Mohanty et al. (1997) used a hybrid sum-junction approach involving two piecewise continuous functions (one of which was a van Genuchten-Mualem type equation).

Several important features of preferential flow can be demonstrated using the variably-saturated dual-permeability model given by Eqs. (17) to (23). Simulation results for infiltration (Gerke & van Genuchten, 1993; van Genuchten & Sudicky, 1999) indicate that equilibrium between the fracture and matrix pore systems should be expected when the hydraulic conductivity function, $K_a(h)$, of the matrix/fracture interface is roughly equal to the conductivity, $K_m(h)$ of the matrix (assuming a fracture spacing of 2 cm). For preferential flow to initiate, K_a had to be much less than K_m . This conclusion is consistent with experimental studies which suggest that a soil aggregate can have a higher local bulk density (and hence lower conductivity) near its surface than in the aggregate center, in part because of the deposition of organic matter, fine-texture mineral particles, or various oxides and hydroxides on the aggregate exteriors or macropore walls. For example, Wilding & Hallmark (1984) noted that ped argillans can markedly reduce rates of diffusion and mass flow from ped surfaces into the soil matrix. Cutans, consisting of coatings with modified physical, chemical or biological properties, often have also preferred orientations parallel to soil aggregate surfaces. Unsaturated fractured rock formations may exhibit similar features, i.e., fracture skins (Moench, 1984), or other types of coatings (Pruess & Wang, 1987; Thoma et al., 1992) made up of fine clay particles, calcite, zeolites or silicates, which may reduce the hydraulic conductivity. Finally, preferential flow within the macropores or fractures themselves can also contribute to a lower effective $K_a(h)$. Situations like this can restrict water and solute exchange between the two pore systems (notably imbibition into the matrix) to only a small portion of the total interface area (Hoogmoed & Bouma, 1980), even in capillary-size pores (Omoti & Wild, 1979). Hydrophobic fracture surfaces can similarly limit fluid exchange between the two pore systems. These various factors likely contributed to the need for Gerke & van Genuchten (1993) to make K_a of the matrix/fracture interface 100 smaller than K_m of the matrix/fracture interface in order to generate significant macropore flow during infiltration. Ho (1997) similarly needed to reduce fracture/matrix interactions by four order of magnitude in order to correctly model infiltration at Yucca Mountain and enable the simulation accurate description of the fast transport of bomb-pulse nuclides.

Hierarchical approach for modeling preferential flow in structured media

The dual-permeability model given by Eqs. (17) through (23) is only one of several approaches that can be used to model flow and/or transport in structured media. Figure 2 shows a schematic of increasingly complex models that may be used to simulate preferential flow. The simplest situation (Fig. 2b) arises when the Richards and advection-dispersion equations (Eqs. 1 and 3) are still used in an equivalent continuum approach, but now with composite hydraulic conductivity (permeability) curves, $K(h)$, of the type shown in Fig. 1a.

More involved dual-porosity type models are obtained when the liquid phase is partitioned into mobile (fracture) and immobile (matrix) liquid pore regions, with water and/or solutes allowed to exchange between the two liquid regions (Fig. 2c). For conditions of steady-state flow this leads to the two dual-porosity formulations given by Eqs. (9) through (11) and (14) through (16). These models could be made more general by permitting transient variably-saturated flow in the fracture, and also by allowing water to exchange between the fracture and matrix domains.

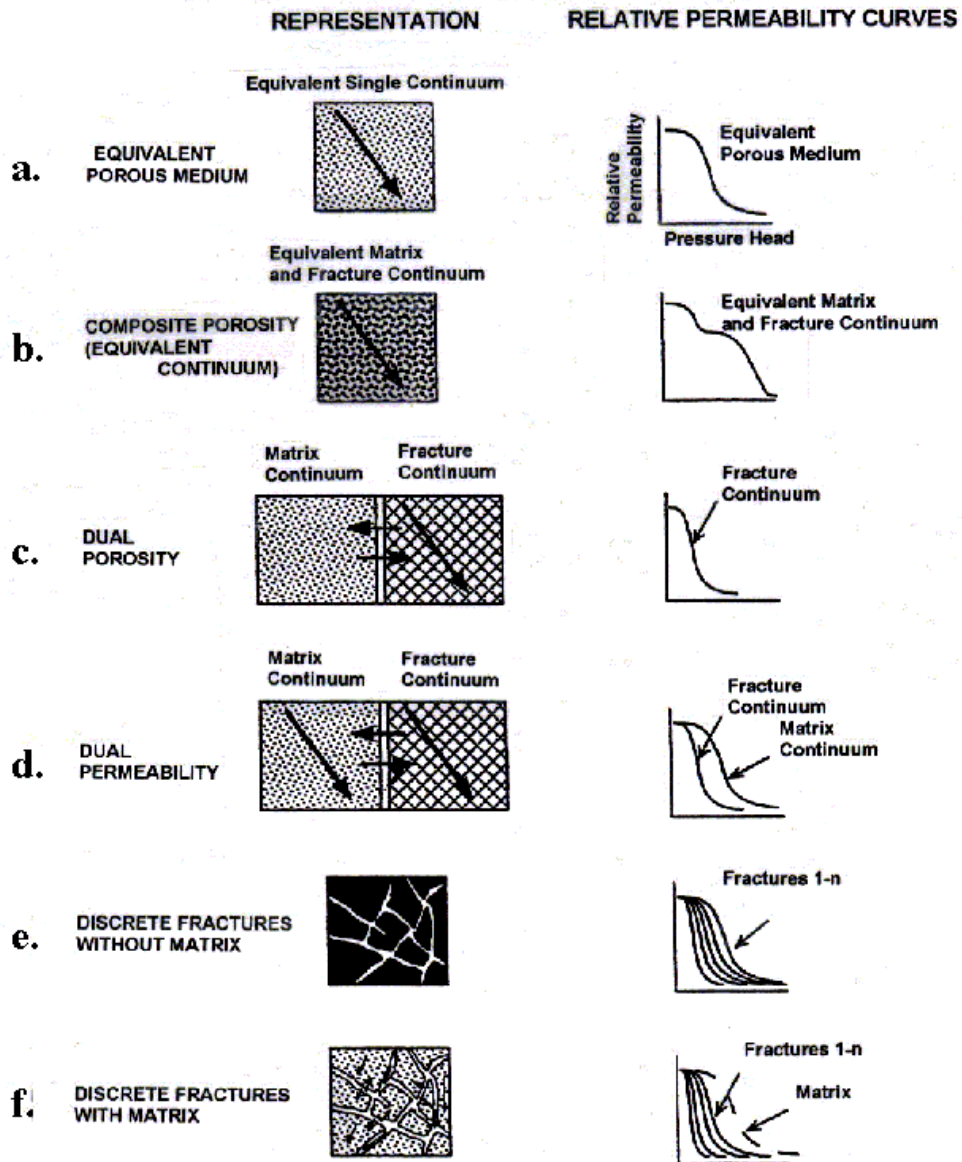


Figure 2. Alternative conceptual models for flow through variably-saturated structured media (after Altman et al., 1996).

The latter dual-porosity situation would lead to both advective and diffusive exchange of solutes between the fracture and matrix regions, but still without vertical flow in the matrix region. Dual-porosity flow/transport models of this type that consider composite hydraulic properties and the presence of immobile water are given by Zurmühl et al. (1998) and Simunek et al. (1999).

More complex dual-permeability models (Fig. 2d) arise when water flow occurs in both the fracture and matrix domains. Examples are models by Gerke and van Genuchten (1993), as described previously by Eqs. (17) through (23), Pruess (1991) and Jarvis (1999). These models all use different formulations for the exchange of water between the fracture and matrix regions. In some models (e.g., Hutson & Wagenet, 1995; Wilson et al., 1999) more than two domains are considered, each one again having its own hydraulic properties.

The modeling approach can be further refined by considering transient variably-saturated flow and/or transport in discrete well-defined fractures, either without (Fig. 2e) or with (Fig. 2f) interactions between the fracture and matrix domains. The approach typically assumes that the flow and transport equations of the macropore or fracture network of prescribed geometry can be solved simultaneously and in a fully-coupled fashion with the corresponding equations for the porous matrix. A discrete-fracture numerical model of this type (Fig. 2f) is given by Shikaze et al. (1994) for two-dimensional gas-phase flow and transport through a network of vadose-zone fractures embedded in a variably-saturated matrix. Another example is given by Therrien & Sudicky (1996) for three-dimensional variably-saturated conditions in which the Richards equation is applied both along a network of interconnected fracture planes, and in the adjoining porous matrix. They superimposed a network of two-dimensional finite elements representing the interconnecting fractures onto the mesh of three-dimensional elements representing the matrix. The fully-coupled approach assumes continuity in the pressure head and the concentration at the fracture/matrix interface, thus permitting a simultaneous solution of the Richards and transport equations for both the fracture network and the porous matrix without a need to explicitly calculate fluxes between the two regions. By applying the Richards equation also to the soil matrix region, the model accounts immediately for water flow into and through the matrix domain.

Application to tile-drainage experiment

We show here one application of the equivalent continuum approach involving composite hydraulic functions and applicability of the standard Richards and advection-dispersion equations (Fig. 2b). The modeling approach is used to data from an experimental tile-drained field site located on a commercial farm in the alluvial flood plain of the Rio Grande near Las Nutrias, New Mexico (Mohanty et al., 1997, 1998). The field site consisted of mostly silty clay loam sediments underlain by fine sands, and with no impeding strata to a depth of about 7 m. The surface horizons contained visible root channels, worm holes, and drying cracks. The site was equipped with surface irrigation and subsurface (tile) drainage systems to reduce salinity in the crop-root zone. Two manholes allowed monitoring of water quantity and quality entering and leaving the study section of the tile drain. Field-averaged hydraulic functions are shown in Figure 1. These functions were incorporated into the CHAIN_2D computer model (Simunek & van Genuchten, 1994) to enable two-dimensional transient simulations at the field site.

One example of simulated tile flow using the field-averaged piecewise-continuous soil hydraulic functions of Figure 1 is presented in Figure 3a and compared against observed values. We also compared the simulation results with results obtained using field-averaged unimodal van Genuchten-Mualem type hydraulic properties. To present a qualitative comparison, we used two unimodal functions for the surface horizon based on (1) $K_{0\text{-cm}}$ through $K_{3\text{-cm}}$ being included in a

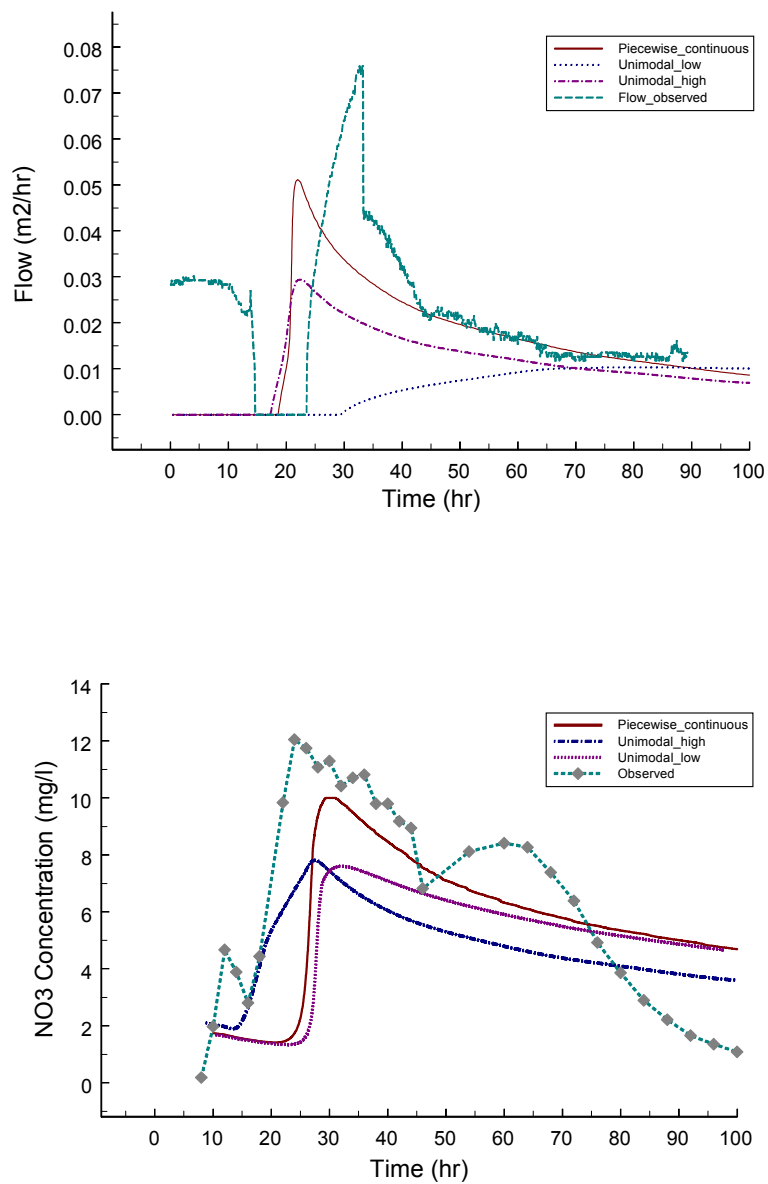


Figure 3. Comparison of observed data with simulated tile-drainage (a) and nitrate concentration (b) distributions using the piecewise-continuous hydraulic functions of Figure 1, as well unimodal van Genuchten-Mualem type hydraulic functions. Time 0 hr matched midnight prior to the flood irrigation event at the Las Nutria field site (after Mohanty et al., 1997, 1998).

parameter optimization analysis of the hydraulic data (unimodal_high), and (2) $K_{0\text{-cm}}$ through $K_{3\text{-cm}}$ being excluded from the analysis (unimodal_low). From the observed tile-drain flow it is clear that, following an irrigation event, water moves rapidly downward through the soil profile. After a few hours of irrigation, the tile flow rate suddenly increased and reached a peak almost instantly followed by a similar sharp drop (these results suggest preferential flow through the field macropore network). This situation was followed by a recession phase dominated by prolonged matrix flow and water redistribution in the profile. In general, predicted flow using the bimodal hydraulic functions matched the observed flow rates reasonably well, and far better than when the unimodal hydraulic functions were used. Figure 3b shows corresponding nitrate transport (simulated vs. observed) at the field site. Further details of this study can be found in Mohanty et al. (1997, 1998).

The piecewise continuous hydraulic functions were reasonably successful in predicting the field-scale flow and transport. Even with these properties, Figure 3a still shows deviations between predicted and measured tile flow rates. We believe that these deviations were caused primarily by the presence of a regional flow field, which may not have been adequately captured with the two-dimensional model that was used. These and other ongoing studies at the U.S. Salinity Laboratory suggest that the use of piecewise-continuous functions, or similar bimodal type hydraulic properties, will lead to better predictions of preferential flow in the vadose zone. Further improvements in the predicted nitrate distributions of Figure 3b should be possible by including provisions for immobile water in the transport equation (e.g., Zurmuhl et al., 1998; Simunek et al., 1999); this should move the leading edge of the nitrate concentration in the tile drain further to the left toward the observed data.

The unsaturated soil hydraulic properties

Application of the variably-saturated flow models to specific field problems requires estimates of the unsaturated soil-hydraulic properties, i.e., the soil water retention, $\theta(h)$, and hydraulic conductivity, $K(h)$, functions in Eq. (1). A large number of laboratory and field methods are available for direct measurement of $\theta(h)$ and $K(h)$ (e.g., Klute, 1986; van Genuchten et al., 1999). Field methods allow for in-situ determination of the hydraulic properties, but have uncertainties about the actual sample volume. Laboratory measurements require more sample preparation but do allow for a larger number of measurements and better control of the experimental conditions. Most laboratory and field techniques, however, have specific ranges of applicability with respect to soil type and saturation (Klute, 1986). Another limitation of direct measurements is that they generally are quite cumbersome and require a substantial investment in both time and money. Also, many vadose zone studies are concerned with relatively large areas of land that may exhibit significant lateral and vertical spatial variability in the soil hydraulic properties. Obtaining adequate direct measurements for these situations is virtually impossible, and alternative indirect methods are needed to generate soil hydraulic properties.

Several useful indirect methods have recently become available. Although these approaches vary widely in terms of methodology and complexity, all use some form of surrogate data to estimate soil hydraulic properties. In broad terms, three methods can be distinguished: pore-size distribution models, inverse methods, and pedotransfer functions.

Pore-size distribution models are often used to estimate the unsaturated hydraulic conductivity from the distribution, connectivity and tortuosity of pores. The pore-size distribution can be inferred from the water retention curve, which is normally much easier to measure than the unsaturated hydraulic conductivity function. One popular model of this type was developed by Mualem (1976) by assuming water flow through cylindrical pores and

incorporating the equations of Darcy and Poiseuille. The model may be simplified into closed-form expressions when the water retention is described with the functions of either Brooks & Corey (1964) or van Genuchten (1980). The latter case leads to the hydraulic functions

$$\theta(h) = \theta_r + \frac{\theta_s - \theta_r}{[1 + |\alpha h|^n]^m} \quad (24)$$

$$K(h) = K_s K_r(h) = K_s S_e^{1/2} [1 - (1 - S_e^{1/m})^m]^2 \quad (25)$$

in which θ_r and θ_s denote the residual and saturated water contents, respectively; K_s is the saturated hydraulic conductivity, K_r is the relative hydraulic conductivity, α and n are shape factors, $m=1-1/n$, and S_e is effective saturation:

$$S_e(h) = \frac{\theta(h) - \theta_r}{\theta_s - \theta_r} \quad (26)$$

The approach above still requires independently measured water retention data as well as an estimate of the saturated hydraulic conductivity, K_s , or some other matching point.

Closed form expressions such as Eqs. (24) and (25) provide a consistent description of the water retention and unsaturated hydraulic conductivity curves, and are convenient for use in numerical models simulating variably-saturated flow. The same set of equations can also be used in inverse problems by combining some numerical solution of the Richards equation with an optimization algorithm to estimate several or all of the unknown parameters K_s , θ_r , θ_s , α and n from observed time series of infiltration, water content and/or pressure head (e.g., Kool et al., 1987; Simunek & van Genuchten, 1996; Abbaspour, 1997). The resulting hydraulic properties may be considered effective properties in that they are obtained from data pertaining to real flow conditions. Unfortunately, inverse methods are often affected by non-uniqueness of the results, i.e., two or more sets of optimized parameters may be applicable to the problem being studied (e.g., Hopmans & Simunek, 1999).

Pedotranfer functions (PTFs, Bouma & van Lanen, 1987) offer a third method for estimating hydraulic properties by using the fact that the hydraulic properties are very much dependent upon soil texture and other readily available soil taxonomic information (e.g., the particle size distribution, bulk density, organic matter content). Several empirical and quasi-empirical PTF approaches exist. Quasi-physical methods such as those by Arya & Paris (1981), Arya et al. (1999) and Haverkamp & Parlange (1986) use the concept of shape similarity between the water retention function and the particle-size distribution. The vast majority of PTFs, however, are completely empirical. Although considerable differences exist among PTFs in terms of the required input data (Rawls et al., 1991), all use at least some information about the particle-size distribution.

Class PTFs assume the same hydraulic properties for similar soils. In this discrete approach one can use lookup tables to find appropriate hydraulic parameters values for a particular soil textural class (e.g., Carsel & Parrish, 1988; Wösten et al., 1995). Continuous PTFs, on the other hand, are based on simple linear or nonlinear regression equations to yield continuously varying hydraulic properties estimates across the textural triangle. The predictions may be improved by adding to the input data such basic soil properties as bulk density, porosity and/or organic matter content (Rawls & Brakensiek, 1985; Vereecken et al. 1989). Additional improvements are possible by including one or more water retention data points in the analysis (Rawls et al., 1992;

Williams et al., 1992). Other authors have predicted soil hydraulic properties using more limited or extended sets of input variables (Rawls et al., 1992; Schaap & Bouten, 1996; Vereecken et al. 1989). Such hierarchical approaches are of great practical use since they permit more flexibility in terms of using all available data.

Recently, neural network analyses have been used to further improve PTF predictions (Pachepsky et al., 1996; Schaap & Bouten, 1996; Tamari et al., 1996). As compared to traditional PTFs, a major advantage of neural networks is that they require no a priori model concept. The optimal, possibly nonlinear, relationships that link input data (such as particle size data or bulk density) to output data (hydraulic parameters) are obtained and implemented in an iterative calibration procedure. As a result, neural network models extract the maximum of information from the data.

One problem with all PTFs is that they provide predictions with a modest level of accuracy (e.g., Tietje & Tapkenhinrichs, 1995). For this reason it is useful to include with the predictions of the hydraulic properties also confidence intervals. To address this issue, and the possible use of different sets of input data, Schaap et al. (1998) used bootstrap-neural network analyses to develop a hierarchical approach for predicting the unknown hydraulic parameters in Eqs. (24) and (25). Five PTFs were developed with data requirements that should suit most practical situations. Use of the bootstrap method (Efron & Tibshirani, 1993) provided confidence intervals for the predictions. Table 2 gives an overview of the required input data for each model, with the root-mean-square residuals (RMSRs) showing the performance of the PTFs on independent data (Schaap et al., 1998). The models were developed using a database containing 2085 samples. Because the same data were used for all models, the predictions should be consistent among each other.

Model 1 in Table 2 is a class PTF; values of the hydraulic parameters for each textural class are shown in Table 3. Models 2 through 5 use more input data to make predictions of soil hydraulic parameters, and thus become progressively more accurate as indicated by the lower RMSR values. Model 2 uses the sand, silt and clay fractions, while Model 3 also requires a measured bulk density value. Models 4 and 5 additionally require one or two retention data points, respectively. Adding observed retention data may seem somewhat counterintuitive since the PTFs eventually will be used to predict water retention. However, the two retention data points referred to in Table 2 are often available in soil survey databases, such as the large NRCS database (Soil Survey Staff, 1995). Using this information leads to much smaller RMSR values

Table 2. Input requirements for five models in the hierarchical PTF approach of Schaap et al. (1998). Root-mean-square residuals (RMSRs) reflect the performance of each model for water retention and the saturated hydraulic conductivity.

Model	Input	Prediction Error (RMSR):	
		Retention [cm ³ cm ⁻³]	K_s [log(cm day ⁻¹)]
Model 1	Textural class	0.108	0.740
Model 2	Sand, silt, clay	0.106	0.735
Model 3	+ bulk density	0.083	0.684
Model 4	+ θ at 33 kPa	0.066	0.611
Model 5	+ θ at 1500 kPa	0.063	0.610

Table 3. Class-average values of the van Genuchten (1980) water retention parameters and the saturated hydraulic conductivity (K_s). N is the number of samples for each textural class.

Textural Class	N	θ_r	θ_s	α	n	K_s
		cm^3/cm^3		1/cm	-	cm/day
Sand	308	0.053	0.375	0.035	3.18	646
Loamy Sand	201	0.049	0.391	0.032	1.76	105
Loam	242	0.062	0.400	0.0098	1.48	12.0
Sandy Loam	476	0.039	0.388	0.026	1.45	38.0
Silt Loam	330	0.065	0.439	0.0049	1.67	18.2
Sandy Clay Loam	172	0.065	0.384	0.017	1.34	13.2
Silty Clay Loam	87	0.090	0.484	0.0076	1.53	11.2
Clay Loam	140	0.083	0.444	0.012	1.44	8.1
Silt*	6	0.050	0.489	0.0066	1.68	43.7
Clay	84	0.100	0.457	0.011	1.27	14.8
Sandy Clay*	11	0.128	0.380	0.025	1.22	11.5
Silty Clay	28	0.115	0.476	0.014	1.33	9.6

*Parameter values may not be reliable because of small number of samples.

than for Model 3 (see Table 1). As shown by Schaap et al. (1998a), neural network predictions can be easily derived also for parameter combinations and input values other than those used for the five models summarized here.

The combination of neural network calibration with the bootstrap method further enables one to quantify model uncertainty on a per sample basis. Figure 4 shows confidence intervals as predicted with Model 3 (Table 2) for the water retention and hydraulic conductivity functions, as well as K_s , for a loamy sand and a clay sample. The figure shows 10 and 90% percentiles of the variability in $\theta(h)$ and $K(h)$, while for K_s the entire probability distribution is given. Notice the much larger uncertainty for the clay soil as compared to the loamy sand. This is caused by the fewer number of fine-textured soils in the data set relative to coarse-textured soils. Uncertainty estimates generally increased when predictions were made for samples that were less common in the calibration data sets (Schaap & Leij, 1998).

The five hierarchical PTFs of Table 2 were implemented in a user-friendly Windows 98 program, called Rosetta. This program allows one to run any of the models of Table 2 for available site-specific data. The program will yield estimates of the parameters θ_r , θ_s , α , n and K_s in Eqs. (24) and (25), as well as estimates of their uncertainties. Having uncertainty estimates of the hydraulic parameters will facilitate probabilistic or risk-based analyses of water and solute transport, among other applications. Version 1.0 of Rosetta is available from the U.S. Salinity Laboratory website (<http://www.ussl.ars.usda.gov/models/Rosetta.htm>).

Concluding remarks

The topics reviewed in this paper should reflect the tremendous advances made during the past several decades in our ability to mathematically describe water and solute movement in the subsurface. Much new information has become available about the underlying processes affecting flow and transport in the subsurface. Simultaneous advances in numerical techniques and computer hardware are now making it increasingly possible to obtain an integrated multidisci-

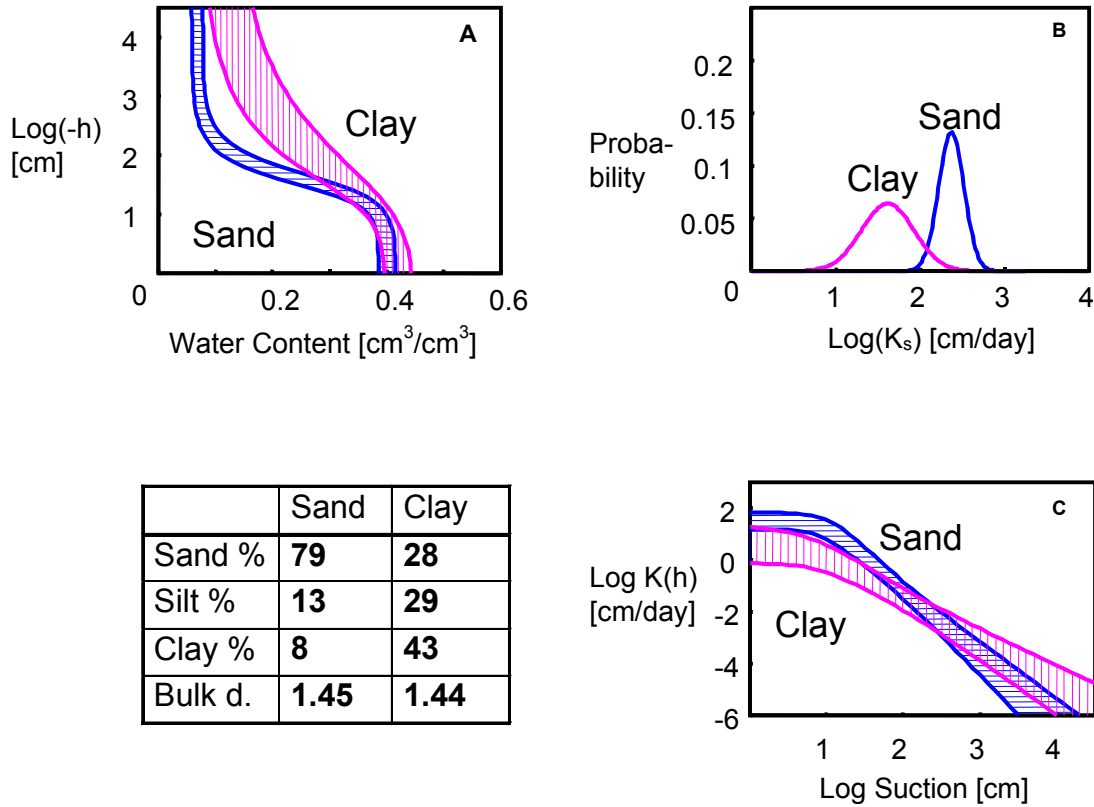


Figure 4. Predictions with uncertainty intervals for the water retention function (A), the saturated hydraulic conductivity (B), and the unsaturated hydraulic conductivity function (C). The table shows input values that were used for the neural network model (Model 3, of Table 1).

plinary description of the vadose zone. New information and related models can now be used to quantify the often controlling effects of heterogeneities, fractures and macropores on flow and transport at the field scale. Accounting for heterogeneity and preferential flow is crucial in studies of agrochemical transport in soils, including investigations of the leaching efficiency of saline soils subjected to different irrigation schemes. Two- and three-dimensional models of the type discussed here are also providing more realistic field- or larger-scale descriptions of transient water and salt movement in irrigation areas. Such models can be especially effective tools for studying the transient behavior of different (tile- or other) drainage systems as compared to the use of more traditional steady-state analytical approaches which only consider water flow.

In spite of the many advances, much remains to be done. Further improvements are necessary in the representation of many underlying physical, chemical and biological processes. Very much needed are improved descriptions of root water uptake, root growth, and transpiration as a function of water and salinity stress; information of this type is needed throughout all stages of plant growth and development. Another important issue is proper field testing of recently developed up-scaling theories for application of models to heterogeneous field systems. Current numerical models designed to predict field-scale flow and chemical transport processes often yield only qualitative similarities to real-world field observations. Attempts to improve the predictive capabilities of recent models have frequently involved the introduction of additional fitting parameters, which are elusive and perhaps impossible to measure independently. This aspect should be a concern given that practitioners, planners, and regulators are increasingly relying upon model predictions to establish far-reaching policies.

A closely related issue is the need for improved methods to estimate relevant soil-hydraulic, transport, chemical, and crop physiology parameters. Designing and conducting long-term field experiments on water and salt movement, including crop growth, can be extremely costly. Some progress is being made in terms of developing computerized relational databases of soil hydraulic properties (Leij et al., 1996) and crop salt-tolerance response information (Ulery et al., 1997). Proper design and careful execution of field experiments often requires thousands of hours of work, and is rapidly becoming prohibitively expensive for individual researchers or even small research institutions. Hence, it is increasingly important that such experiments be properly documented and shared within the scientific and extension communities.

Finally, it is imperative that state-of-the-art numerical models being developed in the research community be shared with, and used more effectively by, soil and groundwater professionals. A tremendous gap still exists between models available within the research community and those used for practical applications in the soil and hydrologic professions (including regulatory agencies). Development of more user-friendly software of appropriate models and databases should narrow this gap.

References

- Abbaspour, K. C., M. Th. van Genuchten, R. Schulin & W. Schlappi, 1997. A sequential uncertainty domain inverse procedure for estimating subsurface flow and transport parameters. *Water Resour. Res.* 33 [8], 1879-1892.
- Altman, S. J., B. W. Arnold, R. W. Barnard, G. E. Barr, C. K. Ho, S. A. McKenna & R. R. Eaton, 1996. Flow calculations for Yucca Mountain groundwater travel time (GWTT-95). SAND96-0819, Sandia National Laboratories, Albuquerque, NM.
- Ankeny, M. D., 1992. Methods and theory for unsaturated infiltration measurements. In: G. Topp et al. (editors), *Advances in Measurement of Soil Physical Properties: Bringing Theory into Practice*. *Soil Sci. Soc. Am. Spec. Publ.* 30, 123-141.
- Arya, L. M. & J. F. Paris, 1981. A physico-empirical model to predict the soil moisture characteristic from particle-size distribution and bulk density data. *Soil Sci. Soc. Am. J.* 45, 218-227.
- Arya, L. M., F. J. Leij, M. Th. van Genuchten & P. J. Shouse, 1999. Scaling parameter to predict the soil water characteristic from particle-size distribution data. *Soil Sci. Soc. Am. J.* 63 [3], 510-519.
- Bolt, G. H. (ed.), 1979. *Soil Chemistry, Physico-Chemical Models*. Elsevier Science, New York, 479 p.
- Bresler, E. & G. J. Hoffman, 1986. Irrigation management for soil salinity control: Theories and tests. *Soil Sci. Soc. Am. J.* 50, 1552-1560.
- Bresler, E., B. L. McNeal & D. L. Carter, 1982. *Saline and Sodic Soils*. Springer Verlag, Berlin.
- Bouma, J. & J. A. J. van Lanen, 1987. Transfer functions and threshold values: From soil characteristics to land qualities. p 106-110. In: K. J. Beek et al. (eds.). *Quantified land evaluation*. International Institute Aerospace Surv. Earth Sci. ITC publ. 6. Enschede, the Netherlands.
- Brooks, R. H. & A.T. Corey, 1964. Hydraulic properties of porous media. *Hydrol. paper* 3, Colorado State Univ., Fort Collins, CO.
- Cardon, G. E. & J. Letey, 1992. Plant water uptake terms evaluated for soil water and solute movement models. *Soil Sci. Soc. Am. J.* 56, 1876-1880.
- Carsel, R. F. & R. S. Parrish, 1988. Developing joint probability distributions of soil water retention characteristics. *Water Resour. Res.* 24, 755-769.

- Darcy, H., 1856. Les Fontaines Publiques de la Ville de Dijon, Dalmont, Paris.
- Durner, W., 1994. Hydraulic conductivity estimation for soils with heterogeneous pore structure. *Water Resour. Res.* 30, 211-223.
- Efron, B. & R. J. Tibshirani, 1993. An Introduction to the bootstrap. Monographs on statistics and applied probability. Chapman and Hall, New York, NY.
- Feddes, R. A., P. J. Kowalik & H. Zaradny, Simulation of Field Water Use and Crop Yield. PUDOC, Wageningen, The Netherlands.
- Gerke, H. H. & M. Th. van Genuchten, 1993. A dual-porosity model for simulating the preferential movement of water and solutes in structured porous media. *Water Resour. Res.* 29 [2], 305-319.
- Gerke, H. H. & M. Th. van Genuchten, 1996. Macroscopic representation of structural geometry for simulating water and solute movement in dual-porosity media. *Adv. Water Resour.* 19[6], 343-357.
- Haverkamp, R. & J. Y. Parlange, 1986. Predicting the water-retention curve from particle size distribution: 1. Sandy soils without organic matter. *Soil Sci.* 142, 325-339.
- Ho, C. K. 1997. Models of fracture-matrix interactions during multiphase heat and mass flow in unsaturated fractured media. In: Sixth Symposium on Multiphase Transport in Porous Media, 1997 ASME Int. Mechanical Engineering Congress and Exposition, Dallas, TX.
- Hoogmoed, W. B. & J. Bouma, 1980. A simulation model for predicting infiltration into cracked clay soil. *Soil Sci. Soc. Am. J.* 44, 458-461.
- Hoffman, G. H. & M. Th. van Genuchten, 1993. Soil properties and efficient water use: Water management for salinity control. In: H. M. Taylor & T. R. Sinclair (eds.), *Limitations to Efficient Water Use in Crop Production*. American Society of Agronomy, Madison, WI.
- Hopmans, J. W. & J. Simunek, 1999. Review of inverse estimation of soil hydraulic properties. In: van Genuchten, M. Th., F. J. Leij, & L. Wu (eds.) *Proc. Int. Workshop, Characterization and Measurement of the Hydraulic Properties of Unsaturated Porous Media*, pp. 643-659, University of California, Riverside, CA.
- Hutson, J. L. & R. J. Wagenet, 1995. A multiregion model describing water flow and solute transport in heterogeneous soils. *Soil Sci. Soc. Am. J.* 59 [3], 743-751.
- Jarvis, N., 1999. Modeling the impact of preferential flow on nonpoint source pollution. In: H. M. Selim and L. Ma (eds.), *Physical Nonequilibrium in Soils: Modeling and Application*. pp. 195-221, Ann Arbor Press, Chelsea, MI.
- Jarvis, N. J. & I. Messing, 1995. Near-saturated hydraulic conductivity in soils of contrasting texture measured by tension infiltrometers. *Soil Sci. Soc. Am. J.* 59, 27-34.
- Klute, A. (ed.), 1986. *Methods of soil analysis, Part 1: Physical and mineralogical methods*, second Edition. Monogr. 9. ASA and SSSA, Madison, WI.
- Kool, J. B., J. C. Parker & M. Th. van Genuchten, 1987. Parameter estimation for unsaturated flow and transport models - a review. *J. Hydrol.* 91, 255-293.
- Leij, F. J., W. J. Alves, M. Th. van Genuchten & J. R. Williams, 1996. The UNSODA unsaturated soil hydraulic database, User's Manual. Version 1.0. EPA/600/R-96/095, National Risk Management Laboratory, Office of Research and Development, U.S. Environmental Protection Agency, Cincinnati, Ohio. (<http://www.ussl.ars.usda.gov/MODELS/UNSODA.HTM>).
- Maas, E. V. & G. J. Hoffman, 1977. Crop salt tolerance - Current assessment. *J. Irrig. Drainage Div. ASCE* 103(IR2), 115-134.
- Mallants, D., P.-H. Tseng, N. Toride, A. Timmerman & J. Feyen, 1997. Evaluation of multimodal hydraulic functions in characterizing a heterogenous field soil. *J. of Hydrol.* 195, 172-199.
- Messing, I. & N. J. Jarvis, 1993. Temporal variation in the hydraulic conductivity of a tilled clay soils as measured by tension infiltrometers. *J. Soil Sci.* 44, 11-24.

- Mohanty, B. P., R. S. Bowman, J. M. H. Hendrickx & M. Th. van Genuchten, 1997. New Piecewise-Continuous Hydraulic Functions for Modeling Preferential Flow in An Intermittent-Flood-Irrigated Field. *Water Resour. Res.* 33, 2049-2063.
- Mohanty, B. P., R. S. Bowman, J. M. H. Hendrickx, J. Simunek & M. Th. van Genuchten, 1998. Preferential Transport of Nitrate to a Tile Drain in an Intermittent-Flood-Irrigated Field: Model Development and Experimental Evaluation. *Water Resour. Res.* 34, 1061-1076.
- Mualem, Y., 1976. A new model for predicting the hydraulic conductivity of unsaturated porous media. *Water Resour. Res.* 12, 513-522.
- Moench, A. F., 1984. Double-porosity models for a fissured groundwater reservoir with fracture skin. *Water Resour. Res.* 20, 831-846.
- Nielsen, D. R., M. Th. van Genuchten & J. W. Biggar, 1986. Water flow and solute transport processes in the unsaturated zone. *Water Resour. Res.* 22 [9], 89s-108s.
- Omoti, U. & A. Wild, 1979. Use of fluorescent dyes to mark the pathways of solute movement through soils under leaching conditions, 1. Laboratory experiments. *Soil Sci.* 128 [4], 28-37.
- Othmer, H., B. Diekkruger & M. Kutilek, 1991. Bimodal porosity and unsaturated hydraulic conductivity. *Soil Sci.* 152, 139-150.
- Pachepsky, Y. A., D. Timlin & G. Varallyay, 1996. Artificial neural networks to estimate soil water retention from easily measurable data. *Soil Sci. Soc. Am. J.* 60, 727-733.
- Peters, R. R., & E. A. Klavetter, 1998. A continuum model for water movement in an unsaturated fractured rock mass. *Water Resour. Res.* 24, 416-430.
- Pruess, K., 1991. Tough2 – A general-purpose numerical simulator for multiphase fluid and heat flow. Rep. LBL-29400, Lawrence Berkeley Laboratory, Berkeley, CA.
- Pruess, K. & J. S. Y. Wang, 1987. Numerical modeling of isothermal and nonisothermal flow in unsaturated-saturated fractured rock- A review. In: Evans D. D. and T. J. Nicholson (eds.), *Flow and Transport Through Unsaturated Fractured Rock*. pp. 11-22, Am. Geophys. Union, Washington, DC.
- Rawls, W. J., T. J. Gish & D. L. Brakensiek, 1991. Estimating soil water retention from soil physical properties and characteristics. In: Stewart, B. A. *Advances in Soil Science*. Springer-Verlag, New York.
- Rawls, W. J. & D. L. Brakensiek, 1985. Prediction of soil water properties for hydrologic modeling. p 293-299. In: Jones, E. B. & T. J. Ward (ed.) *Watershed management in the eighties*. Proc. Irrig. Drain. Div. ASCE, Denver, CO. April 30 - May 1. 1985.
- Rawls, W. J., L. R. Ahuja & D. L. Brakensiek, 1992. Estimating soil hydraulic properties from soils data. p 329-340. In M. Th. van Genuchten, F. J. Leij, & L. J. Lund (ed.). *Indirect methods for estimating the hydraulic properties of unsaturated soils*. Proc. Int Worksh. Riverside, CA. Oct 11-13. 1989. University of California, Riverside, CA.
- Richards, L. A., 1931. Capillary conduction of liquids through porous media. *Physics* 1, 318-333.
- Ritsema, C. J., L. W. Dekker, J. H. M. Hendrickx & W. Hamminga, 1993. Preferential flow mechanism in a water repellent soil. *Water Resour. Res.* 29, 2183-2193.
- Russo, D., 1988. Determining soil hydraulic properties by parameter estimation: On the selection of a model for the hydraulic properties. *Water Resour. Res.* 24, 453-459.
- Schaap, M. G. & W. Bouten, 1996. Modeling water retention curves of sandy soils using neural networks. *Water Resour. Res.* 32, 3033-3040.
- Schaap, M. G. & F. J. Leij, 1998. Database related accuracy and uncertainty of pedotransfer functions. *Soil Science* 163, 765-779.

- Schaap, M. G., F. J. Leij & M. Th. van Genuchten, 1998. Neural network analysis for hierarchical prediction of soil water retention and saturated hydraulic conductivity. *Soil Sci. Soc. Am. J.* 62, 847-855.
- Shikaze, S. G., E. A. Sudicky & C. A. Mendoza, 1994. Simulation of dense vapor migration in discretely fractured geologic media. *Water Resour. Res.* 30 [7], 1993-2009.
- Simunek, J. & D. L. Suarez, 1993. The UNSATCHEM_2D code for simulating two-dimensional variably-saturated water flow, heat transport, carbon dioxide transport and solute transport with major ion equilibrium and kinetic chemistry. Version 1.1, Research Report No. 128, U.S. Salinity Laboratory, USDA, ARS, Riverside, CA.
- Simunek, J. & D. L. Suarez, 1994. Two-dimensional transport model for variably saturated porous media with major ion chemistry. *Water Resour. Res.* 30 [4], 1115-1133.
- Simunek, J. & M. Th. van Genuchten, 1994. The CHAIN_2D code for simulating the two-dimensional movement of water, heat and multiple solutes in variably saturated porous media. Version 1.1, Research Report No. 136, U.S. Salinity Laboratory, USDA, ARS, Riverside, CA.
- Simunek, J., D. L. Suarez & M. Sejna, 1996. The UNSATCHEM software package for simulating one-dimensional variably saturated water flow, heat transport, carbon dioxide production and transport, and multicomponent solute transport with major ion chemistry. Version 2.0, Research Report No. 141, U.S. Salinity Laboratory, USDA, ARS, Riverside, CA.
- Simunek, J. & M. Th. van Genuchten, 1996. Estimating unsaturated soil hydraulic properties from tension disc infiltrometer data by numerical inversion. *Water. Resour. Res.* 32, 2683-2696.
- Simunek, J. & D. L. Suarez, 1997. Sodic soil reclamation using multicomponent transport modeling. *J. Irrig. Drainage Div. ASCE* 123 [5], 367-376.
- Simunek, J., M. Sejna & M. Th. van Genuchten, 1999. The HYDRUS-2D Software package or simulating the one-dimensional movement of water, heat and multiple solutes in variably-saturated media. IGWMC-TPS 53, Version 2.0. Int. Ground Water Modeling Center, Colorado School of Mines, Golden, CO.
- Smettem, K. R. J. & C. Kirby, 1990. Measuring the hydraulic properties of stable aggregated soil. *J. Hydrol.* 117, 1-13.
- Suarez, D. L. & J. Simunek, 1993. Modeling of carbon dioxide transport and production in soil: 2. Parameter selection, sensitivity analysis and comparison of model predictions to field data. *Water Resour. Res.* 29, 499-513.
- Suarez, D. L. & J. Simunek, 1996. Solute transport modeling under variably saturated flow conditions. In: Lichtner, P. C., C. I. Seefel & E. H. Oelkers (eds), *Reactive Transport in Porous Media, Reviews in Mineralogy*, Vol. 34, Mineral. Soc. Am., Washington, DC, pp.229-268.
- Soil Survey Staff, 1995. Soil survey laboratory information manual. *Soil Surv. Invest. Rep. no 45*. Natl. Soil Surv. Center, Lincoln, NE.
- Tamari, S., J. H. M. Wösten & J. C. Ruiz-Suárez, 1996. Testing an artificial neural network for predicting soil hydraulic conductivity. *Soil Sci. Soc. Am. J.* 60, 1732-1741.
- Therrien, R. & E. A. Sudicky, 1996. Three-dimensional analysis of variably-saturated flow and solute transport in discretely-fractured porous media. *J. Contam. Hydrol.* 23, 1-44.
- Thoma, S. G., D. P. Gallegos & D. M. Smith, 1992. Impact of fracture coatings on fracture/matrix flow interactions in unsaturated, porous media. *Water Resour. Res.* 28, 1357-1367.
- Tietje, O. & M. Tapkenhinrichs, 1993. Evaluation of pedotransfer functions. *Soil Sci. Soc. Am. J.* 57, 1088-1095.
- Ulery, A. L., J. A. Teed, M. Th. van Genuchten & M. C. Shannon, 1997. SALT_TOL_DB: A database of plant yield response to salinity. *Agron. J.* 90 [4], 556-562.

- van Genuchten, M. Th., 1980. A closed-form equation for predicting the hydraulic conductivity of unsaturated soils. *Soil Sci. Soc. Am. J.* 44, 892-898.
- van Genuchten, M. Th., 1985. A general approach for modeling solute transport in structured soils. *Proc. 17th. Int. Congress, Hydrogeology of Rocks of Low Permeability. Jan. 7-11, Tucson, AZ, Memoires Int. Assoc. Hydrogeol.* 17 [2], 513-526.
- van Genuchten, M. Th. & F. N. Dalton, 1986. Models for simulating salt movement in aggregated field soils. *Geoderma* 38, 165-183.
- van Genuchten, M. Th., D. L. Suarez & M. C. Shannon, 1997. Modeling solute transport in salt-affected irrigated soils. In: *Int. Conference on Water Quality Management, Salinity and Pollution Control Towards Sustainable Irrigation in the Mediterranean Region, Vol. I*, pp. 181-200, Sept. 22-26, 1997, Instituto Mediterraneo, Bari, Italy.
- van Genuchten, M. Th., 1987. A numerical model for water and solute movement in and below the root zone. Unpublished Research Report, U. S. Salinity Laboratory, USDA, ARS, Riverside, CA.
- van Genuchten, M. Th. & S. K. Gupta, 1993. A reassessment of the crop salt tolerance response function. *J. Indian Soc. Soil Sci.* 41 [4], 730-737.
- van Genuchten, M. Th. & E. A. Sudicky, 1999. Recent advances in vadose zone flow and transport modeling. In: *Parlange M. B. & J. W. Hopmans (eds), Vadose Zone Hydrology: Cutting Across Disciplines*, Oxford University Press, pp. 155-193.
- van Genuchten, M. Th., F. J. Leij & L. Wu (eds.), 1999. *Proc. Int. Workshop, Characterization and Measurement of the Hydraulic Properties of Unsaturated Porous Media*, University of California, Riverside, CA.
- Vereecken, H., J. Maes, J. Feyen & P. Darius, 1989. Estimating the soil moisture retention characteristic from texture, bulk density, and carbon content. *Soil Sci.* 148, 389-403.
- Wang, Z., J. Feyen, D. R. Nielsen & M. Th. van Genuchten, 1997. Two-phase flow infiltration equations accounting for air entrapment effects. *Water Resour. Res.* 33 [12], 2759-2767.
- Wilding, L. P. & C. T. Hallmark., 1984. Development of structural and microfabric properties in shrinking and swelling clays. In: *Bouma J. & P. A. C. Raats (eds.), Proc. ISSS Symposium on Water and Solute Movement in Heavy Clay Soils, Publ. 37*, pp. 1-18, Int. Inst. for Land Reclamation and Improvement, Wageningen, The Netherlands.
- Williams, R. D., L. R. Ahuja & J. W. Naney, 1992. Comparison of methods to estimate soil water characteristics from limited texture, bulk density, and limited data. *Soil Sci.* 153, 172-184.
- Wilson, G. V., P. M. Jardine & J. P. Gwo, 1992. Modeling the hydraulic properties of a multiregion soil. *Soil Sci. Soc. Am. J.* 56, 1731-1737.
- Wösten J. H. M., P. A. Finke & M. J. W. Jansen, 1995. Comparison of class and continuous pedotransfer functions to generate soil hydraulic characteristics. *Geoderma* 66, 227-237.
- Zimmerman, R. W., G. Chen, T. Hadgu & G. S. Bodvarsson, A numerical dual-porosity model with semianalytical treatment of fracture/matrix flow. *Water Resour. Res.* 29 [7], 2127-2137, 1993.
- Zurmhhl, T., 1998. Capability of convection-dispersion transport models to predict transient water and solute movement in undisturbed columns. *J. Contaminant Hydrology* 30, 101-128.
- Zurmhhl, T. & W. Durner, 1996. Modeling transient water and solute transport in a biporous soil. *Water Resour. Res.* 32, 819-829.