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# Review and comparison of models for describing non-equilibrium and preferential flow and transport in the vadose zone

Jirka Šimůnek<sup>a,\*</sup>, Nick J. Jarvis<sup>b,1</sup>, M.Th. van Genuchten<sup>a</sup>, Annemieke Gärdenäs<sup>b</sup>

<sup>a</sup>George E. Brown Jr. Salinity Laboratory, USDA-ARS, 450 West Big Springs Road, Riverside, CA 92507, USA

<sup>b</sup>Department of Soil Sciences, Swedish University of Agricultural Sciences, P.O. Box 7014, 750 07 Uppsala, Sweden

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## Abstract

In this paper, we review various approaches for modeling preferential and non-equilibrium flow and transport in the vadose zone. Existing approaches differ in terms of their underlying assumptions and complexity. They range from relatively simplistic models to more complex physically based dual-porosity, dual-permeability, and multi-region type models. A relatively simple dual-porosity flow model results when the Richards equation is combined with composite (double-hump type) equations for the hydraulic properties to account for both soil textural (matrix) and soil structural (fractures, macropores, ped) effects on flow. The simplest non-equilibrium flow model, a single-porosity model which distinguishes between actual and equilibrium water contents, is based on a formulation by Ross and Smettem [Soil Sci. Soc. Am. J. 64 (2000) 1926] that requires only one additional parameter to account for non-equilibrium. A more complex dual-porosity, mobile-immobile water flow model results when the Richards or kinematic wave equations are used for flow in the fractures, and immobile water is assumed to exist in the matrix. We also discuss various dual-permeability models, including the formulation of Gerke and van Genuchten [Water Resour. Res. 29 (1993a) 305] and the kinematic wave approach as used in the MACRO model of Jarvis [Technical Description and Sample Simulations, Department of Soil Science, Swedish University of Agricultural Science, Uppsala, Sweden (1994) 51]. Both of these models invoke terms accounting for the exchange of water and solutes between the matrix and the fractures. Advantages and disadvantages of the different models are discussed, and the need for inter-code comparison is stressed, especially against field data that are sufficiently comprehensive to allow calibration/validation of the more complex models and to distinguish between alternative modeling concepts. Several examples and comparisons of equilibrium and various non-equilibrium flow and transport models are also provided.

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**Keywords:** Preferential flow; Non-equilibrium flow; Vadose zone; Dual-porosity models; Dual-permeability models; Solute transport; Pedon scale

## 1. Introduction

The problem of non-equilibrium and/or preferential flow and transport has received much attention in the soil and agricultural sciences because of its implications in accelerating the movement of agricultural contaminants (fertilizers, pesticides,

\* Corresponding author. Tel.: +1-909-369-4865; fax: +1-909-342-4964.

E-mail addresses: [jsimunek@ussl.ars.usda.gov](mailto:jsimunek@ussl.ars.usda.gov) (J. Šimůnek), [nick.jarvis@mv.slu.se](mailto:nick.jarvis@mv.slu.se) (N.J. Jarvis).

<sup>1</sup> Tel.: +46-18-67-2465; fax: +46-18-67-2795.

pathogenic microorganisms, toxic trace elements) through the unsaturated zone to underlying groundwater. The potentially rapid migration of radionuclides from low- and high-level nuclear waste disposal facilities, and the preferential movement of non-aqueous liquids or other pollutants from underground storage tanks, waste disposal sites and mine tailings, has also become a concern for hydrologists, geophysicists, and environmental scientists.

Preferential and non-equilibrium flow and transport are probably the most frustrating processes in terms of hampering accurate predictions of contaminant transport in soils and fractured rocks. Preferential flow, as opposed to uniform flow, results in irregular wetting of the soil profile as a direct consequence of water moving faster in certain parts of the soil profile than in others. [Hendrickx and Flury \(2001\)](#) defined preferential flow as ‘all phenomena where water and solutes move along certain pathways, while bypassing a fraction of the porous matrix’. Thus, an important characteristic of preferential flow is that during wetting, part of the moisture front can propagate quickly to significant depths while bypassing a large part of the matrix pore-space. Water and solutes may move to far greater depths, and much faster, than would be predicted with the Richards equation using area-averaged moisture contents and pressure heads ([Beven, 1991](#)). Another important characteristic of preferential (non-uniform) flow is its non-equilibrium nature. Even for uniform flow conditions, most of the water and its dissolved solutes generally move through the largest continuous pores that are filled with water at a particular tension. This is reflected in the shape of the highly non-linear hydraulic conductivity function, which typically shows dramatic increases with increasing water contents, particularly as the larger pores become active. While conditions at or close to equilibrium exist between the different types of pores in a soil during uniform flow, this is generally not the case during preferential flow. Following the ideas developed by [Skopp \(1981\)](#) and [Flühler et al. \(1996\)](#), [Jarvis \(1998\)](#) considered non-equilibrium to be the most important feature of preferential flow by defining it as a flow regime in which ‘for various reasons, infiltrating water does not have sufficient time to equilibrate with slowly moving resident water in the bulk of the soil matrix’.

The presence of macropores and other structural features, development of flow instabilities (i.e. fingering) caused by profile heterogeneities or water repellency ([Hendrickx et al., 1993](#)), and funneling of flow due to the presence of sloping soil layers that redirect downward water flow are probably the most important causes of preferential flow. While the latter two processes, i.e. flow instability and funneling, are usually caused by textural differences and other factors at scales significantly larger than the pore-scale, macropore flow and transport are usually generated at pore or slightly larger scales, including scales where soil structure first manifests itself (i.e. the pedon scale). Following a recent report by [NRC \(2001\)](#), we will use the term granular medium to refer to those media in which flow and transport are not significantly affected by the presence of macropores and fractures, and in which infiltration produces relatively uniform wetting fronts.

The last two decades have seen the development of a relatively large number of models that consider non-equilibrium flow. In this paper, we review several popularly used approaches to modeling preferential and non-equilibrium flow and transport in the vadose zone starting with relatively simplistic approaches, followed by models of increasing complexity. While [Hendrickx and Flury \(2001\)](#) discussed preferential flow mechanisms and processes at various scales, from pore to areal scales, in this paper we will focus mainly on models describing macropore and non-equilibrium flow resulting from processes at the pore to pedon scales.

## 2. Conceptual models

Preferential flow in structured media (both macroporous soils and fractured rocks) can be described using a variety of dual-porosity, dual-permeability, multi-porosity, and/or multi-permeability models ([Pruess and Wang, 1987](#); [Gerke and van Genuchten, 1993a](#); [Gwo et al., 1995](#); [Jarvis, 1998](#)). Dual-porosity and dual-permeability models both assume that the porous medium consists of two interacting regions, one associated with the inter-aggregate, macropore, or fracture system, and one comprising micropores (or intra-aggregate pores) inside soil aggregates or the rock matrix. While dual-porosity models assume that

water in the matrix is stagnant, dual-permeability models allow for water flow in the matrix as well.

Dual-porosity models have long been applied to solute transport studies. Especially popular early on were dual-porosity models in which distinct mobile and immobile flow regions are assumed to be present (van Genuchten and Wierenga, 1976). Dual-permeability models in which water can move in both the inter- and intra-aggregate pore regions are now also becoming more popular (Pruess and Wang, 1987; Gerke and van Genuchten, 1993a; Jarvis, 1994). Available dual-permeability models differ mainly in how they implement water flow in and between the two pore regions, especially with respect to the degree of simplification and empiricism. Approaches to calculating water flow in macropores or inter-aggregate pores range from those invoking Poiseuille's equation (Ahuja and Hebson, 1992), the Green and Ampt or Philip infiltration models (Ahuja and Hebson, 1992; Chen and Wagenet, 1992), the kinematic wave equation (Germann, 1985; Germann and Beven, 1985; Jarvis, 1994), and the Richards equation (Gerke and van Genuchten, 1993a). Multi-porosity and/or multi-permeability models are based on the same concept as dual-porosity and dual-permeability models, but include additional interacting pore regions (Gwo et al., 1995; Hutson and Wagenet, 1995). They can be simplified immediately to dual-porosity/permeability models.

### 3. Equilibrium flow and transport models

Process-based models for flow and transport in granular (or single-porosity) media are generally based on the Richards equation for variably saturated water flow and the convection–dispersion equation for solute transport, i.e.:

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

$$\begin{aligned} \frac{\partial \theta c}{\partial t} + \frac{\partial \rho s}{\partial t} &= \frac{\partial}{\partial z} \left( \theta D \frac{\partial c}{\partial z} \right) - \frac{\partial qc}{\partial z} - \mu(\theta c + \rho s) \\ &+ \gamma \theta + \gamma \rho \end{aligned} \quad (2)$$

respectively, where  $z$  is the vertical coordinate (positive upwards),  $t$  is time,  $S$  is a sink term,  $h$  is

the pressure head,  $\theta$  is the water content,  $K$  is the unsaturated hydraulic conductivity function,  $c$  and  $s$  are solute concentrations in the liquid and solid phases, respectively,  $q$  is the volumetric flux density,  $\mu$  is a first-order rate constant,  $\gamma$  is a zero-order rate constant,  $\rho$  is the soil bulk density, and  $D$  is the dispersion coefficient. For convenience, we will lump below all zero- and first-order rate reactions into one term,  $\phi$ . Eq. (1) is invariably accompanied by a set of constitutive relations characterizing the unsaturated soil hydraulic properties, specifically the retention curve,  $\theta(h)$ , and the unsaturated hydraulic conductivity function,  $K(h)$ . Commonly used soil hydraulic models for granular media were reviewed by Leij et al. (1997).

Although Eqs. (1) and (2) by themselves generally describe uniform flow and transport, they often also appear in various modifications, and/or have been combined with other expressions or assumptions, to yield alternative approaches accounting for non-equilibrium preferential flow. Eqs. (1) and (2) are, for example, often used to describe flow and transport in individual pore domains of dual- and multi-permeability models.

#### 3.1. Composite retention and hydraulic conductivity functions

A very simple dual-porosity flow model results when the Richards equation is combined with double-hump type composite equations for the hydraulic properties. For example, Othmer et al. (1991) and Durner (1994) divided the porous medium into two (or more) overlapping regions and suggested to use for each of these regions a van Genuchten–Mualem type function (van Genuchten, 1980) of the soil hydraulic properties. Linear superposition of the functions for each particular region gives the functions for the entire multi-modal pore system (Durner et al., 1999):

$$S_e(h) = \frac{\theta(h) - \theta_r}{\theta_s - \theta_r} = \sum_{i=1}^k w_i \frac{1}{(1 + |\alpha_i h|^{m_i})^{m_i}} \quad (3)$$

$$K(\theta) = K_s \left( \sum_{i=1}^k w_i S_{e_i} \right)^l \frac{\left( \sum_{i=1}^k w_i \alpha_i [1 - (1 - S_{e_i}^{1/m_i})^{m_i}] \right)^2}{\left( \sum_{i=1}^k w_i \alpha_i \right)^2} \quad (4)$$

where  $S_e$  is the effective water content, and  $\theta_r$  and  $\theta_s$  denote the residual and saturated water contents, respectively. The integer  $k$  denotes the number of overlapping subregions,  $w_i$  are the weighting factors for the sub-curves, and  $\alpha_i$ ,  $n_i$ ,  $m_i$  ( $1 - 1/n_i$ ), and  $l$  are empirical parameters of the sub-curves. The hydraulic characteristics defined by Eqs. (3) and (4) contain  $4 + 2k$  unknown parameters:  $\theta_r$ ,  $\theta_s$ ,  $\alpha_i$ ,  $n_i$ ,  $l$ , and  $K_s$ . Of these,  $\theta_r$ ,  $\theta_s$ , and  $K_s$  have a physical meaning, whereas  $\alpha_i$ ,  $n_i$ , and  $l$  are essentially empirical parameters determining the shape of the retention and hydraulic conductivity functions (van Genuchten, 1980).

An example of the composite retention and hydraulic conductivity functions for two overlapping porous media is shown in Fig. 1. Note that the pressure head axes are on a log scale, which causes the near-saturated values to be significantly enlarged. In this example, the fracture domain represents only 2.5% of the entire pore-space, but it accounts for almost 90% of the hydraulic conductivity close to saturation. Curves similar to those in Fig. 1 have been used also for fractured rock by Peters and Klavetter (1988), Pruess and Wang (1987), and Flint et al. (2001), among others.

One example of piecewise continuous ('cut and join' type) functions that account for a rapid increase in the hydraulic conductivity near saturation was proposed by Mohanty et al. (1997) who used a van Genuchten–Mualem model for the capillary-dominated flow domain and the following exponential function to account for the non-capillary-dominated flow domain

$$K(h) = K^* + K^* [e^{(h-h^*)\delta} - 1] \quad h^* < h \leq 0 \quad (5)$$

where  $h^*$  is the critical or breakpoint soil water pressure head where flow changes from capillary-dominated to non-capillary-dominated flow,  $K^*$  is the hydraulic conductivity corresponding to  $h^*$ , and  $\delta$  is a fitting parameter representing effective macroporosity or other structural features contributing to non-capillary-dominated flow. Very similar exponential functions to account for the increase in hydraulic conductivity due to macropores in the near-saturated water content range have been used by Smettem et al. (1991) and Ross and Smettem (2000), among others.

A slightly different description was used by Šimůnek et al. (1998, 1999a) in the HYDRUS models and its predecessors to account for rapid increases in the conductivity near saturation as a result of macropore flow. Capillary-dominated flow was described using the van Genuchten–Mualem model for the unsaturated hydraulic conductivity at lower water contents until some point ( $h_k$ ,  $K_k$ ), while a linear increase in conductivity was assumed between this point and saturation to account for non-capillary, macropore-dominated flow (Vogel and Císlerová, 1988). Examples of applications that used composite functions to account for increases in the hydraulic conductivity close to saturation are given by Smettem et al. (1991), Mohanty et al. (1997, 1998), de Vos et al. (1999), and Šimůnek and de Vos (1999).

Although composite hydraulic functions of the type discussed earlier can account for a significant increase in the hydraulic conductivity near saturation, they do not by themselves lead to preferential flow. When used in a single-domain model based on the Richards equation, simulations will still produce uniform wetting fronts, although possibly with some

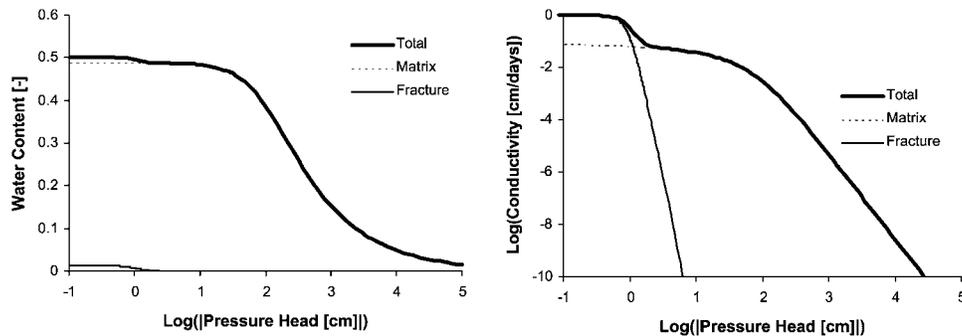


Fig. 1. Example of composite retention (left) and hydraulic conductivity (right) functions ( $\theta_r = 0.00$ ,  $\theta_s = 0.50$ ,  $\alpha_1 = 0.01 \text{ cm}^{-1}$ ,  $n_1 = 1.50$ ,  $l = 0.5$ ,  $K_s = 1 \text{ cm d}^{-1}$ ,  $w_1 = 0.975$ ,  $w_2 = 0.025$ ,  $\alpha_2 = 1.00 \text{ cm}^{-1}$ ,  $n_2 = 5.00$ ).

accelerated advance of the front for surface ponding conditions because of the higher saturated conductivity. Such models, however, cannot predict preferential flow since there is no mechanism to account for lateral non-equilibrium in terms of water moving primarily through larger pores or fractures and bypassing the matrix pore-space. Models based on composite hydraulic property functions implicitly assume instantaneous equilibrium (i.e. instantaneous exchange of water) between the two pore systems. Also, double-hump type equations are typical of soils having bimodal pore-size distributions, which can, but does not necessarily have to, be a dual-porosity medium exhibiting non-equilibrium preferential flow.

#### 4. Non-equilibrium flow and transport models

##### 4.1. Single-porosity models

A relatively simple non-equilibrium flow model was recently proposed by Ross and Smettem (2000). Their model is based on observations in the literature (Schultze et al., 1999; Wildenschild et al., 2001) that water contents may sometimes differ greatly from those given by the equilibrium retention curve, especially during rapid flow, and that equilibrium may be reached only slowly as time proceeds. Ross and Smettem (2000) took this non-equilibrium process into account by combining the classical Richards equation (1) with a kinetic description for the water content approach towards equilibrium. By doing so they removed from the Richards equation the assumption that water contents and pressure heads are tightly coupled through the equilibrium retention curve. Since decoupling of the pressure head and the water content in Eq. (1) now leads to two independent variables ( $h$  and  $\theta$ ), they replaced the equilibrium coupling assumption by an additional differential equation:

$$\frac{\partial \theta}{\partial t} = f(\theta, \theta_e) \quad (6)$$

where  $f(\theta, \theta_e)$  is a known function of the actual and equilibrium water contents. Ross and Smettem (2000) assumed a simple linear driving function for  $f$ , i.e.  $f(\theta, \theta_e) = (\theta_e - \theta)/\tau$ , where  $\tau$  is an equilibration time constant. Substituting this function into Eq. (6),

approximating the resulting expression by an implicit finite difference equation, and incorporating this into their numerical model produced the following approximation (Ross and Smettem, 2000):

$$\theta^{j+1} = \theta^j + (\theta_e^{j+1} - \theta^j)[1 - \exp(-\Delta t/\tau)] \quad (7)$$

where the superscripts  $j + 1$  and  $j$  represent the new and old time levels in the numerical time discretization and  $\Delta t$  is time step. Although one could undoubtedly formulate more sophisticated non-equilibrium models, an important advantage of Eq. (7) is that it requires only one additional parameter to account for non-equilibrium. Another advantage is that it can be implemented easily into existing variably saturated flow models, especially those based on the mixed formulation of the Richards equation. However, when we incorporated Eq. (7) in the HYDRUS models (Šimůnek et al., 1998, 1999a) we experienced some numerical instabilities for relatively large values of the time constant  $\tau$  when the non-equilibrium moisture front moves rapidly through the medium (i.e. when large changes in the pressure head produce only small changes in the water content). One disadvantage of this approach is that the level of preferential flow being produced is independent of the current water content (i.e. antecedent water content).

Ross and Smettem (2000) used Eq. (7) to successfully simulate constant flux infiltration and outflow responses for six large undisturbed cores. We also used the model to successfully describe upward infiltration data on small-undisturbed soil samples (Šimůnek et al., 2001) that exhibited severe non-equilibrium between measured pressure heads and volumes of infiltrated water.

When using Ross and Smettem (2000) model, an interesting question is how to best evaluate the hydraulic conductivity, i.e. as a function of the pressure head,  $h$ , or the water content,  $\theta$ . Note, again, that  $\theta$  and  $h$  now are uncoupled and thus the relation between them is not unique. For the calculations discussed later, we followed Ross and Smettem (2000) by calculating the hydraulic conductivity as a function of the pressure head. This implicitly introduces the assumption that water will move, contrary to assumptions inherent in the Richards equation, first through the larger pores that

dominate the overall hydraulic conductivity. Calculating the hydraulic conductivity as a function of the water content would significantly reduce the non-equilibrium features of this formulation.

Fig. 2 compares pressure head and water content profiles calculated using the equilibrium (Eq. (1)) and Ross and Smettem non-equilibrium (Eq. (7)) water flow models. Van Genuchten (1980) soil hydraulic parameters for a loamy soil ( $\theta_r = 0.02$ ,  $\theta_s = 0.35$ ,  $\alpha_1 = 0.041 \text{ cm}^{-1}$ ,  $n_1 = 1.96$ ,  $l = 0.5$ ,  $K_s = 0.000722 \text{ cm s}^{-1}$ ) were used in the simulations. Ponding ( $h = 1 \text{ cm}$ ) was assumed at the soil surface and the initial pressure head was set equal to  $-150 \text{ cm}$ . A value of  $3600 \text{ s}$  was used for the time constant,  $\tau$ , in the non-equilibrium model. Depending

upon the value of  $\tau$ , this model can produce wetting fronts that will travel initially much faster, and to greater depths (Fig. 2(b)), than those produced with the equilibrium flow model (Fig. 2(a)). The wetting front reached a depth of  $35 \text{ cm}$  after  $1800 \text{ s}$  for the non-equilibrium model (Fig. 2(b)), as opposed to a depth of only  $15 \text{ cm}$  for the equilibrium model (Fig. 2(a)). This much deeper penetration is caused by the fact that flow initially is restricted to only a small part of the flow domain (Fig. 2(b)). The wetting front will eventually advance much slower since most of the infiltrating water is later used for increasing the water content behind the wetting front towards equilibrium (Fig. 2(b)), rather than for more downward vertical flow. For this reason, the moisture

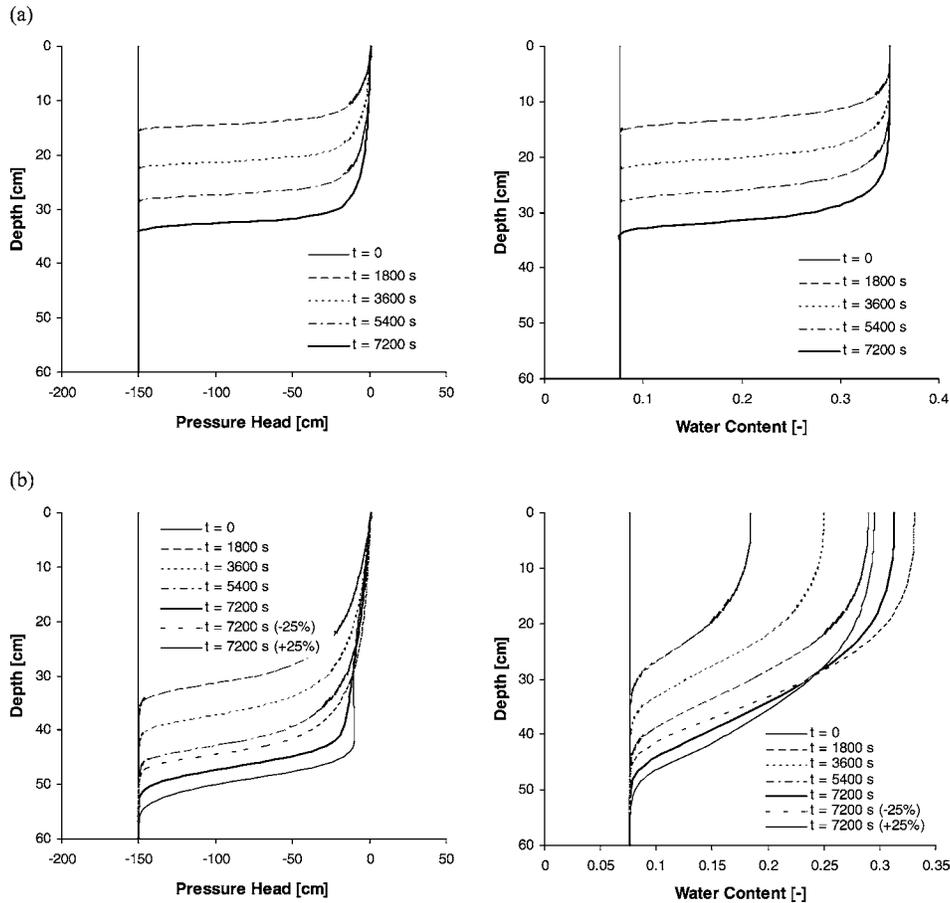


Fig. 2. Pressure head and water content profiles calculated with the (a) equilibrium (Eq. (1)) and (b) non-equilibrium (Eq. (7)) (Ross and Smettem, 2000) water flow models. Thin lines in (b) represent final profiles ( $t = 7200 \text{ s}$ ) when the equilibration time constant,  $\tau$ , is decreased or increased by 25%.

front advanced only 20 cm between 1800 and 7200 s, for both the equilibrium and non-equilibrium models. In order to demonstrate the sensitivity of the Ross and Smettem model predictions to the equilibration time constant,  $\tau$ , we included into Fig. 2(b) the final pressure head and water content profiles ( $t = 7200$  s) obtained when we decreased or increased  $\tau$  by 25% (i.e.  $\tau = 2700$  and 4500 s, respectively).

When the non-equilibrium model of Ross and Smettem (2000) is coupled with the classical convection–dispersion equation (2), the solute front will move much slower than the moisture front because of the assumption that incoming water completely mixes with water initially stored in the profile (Fig. 3(b)). This complete mixing produces concentration profiles that are very similar to those obtained using the equilibrium description for water flow (Fig. 3(a)). Hence, to produce rapidly moving solute fronts, one must also invoke assumptions for non-equilibrium transport, such as the presence of immobile water (Fig. 3(c)). This feature will be discussed in a later section. For the calculations shown in Fig. 3, water flow was the same as for Fig. 2, the dispersivity was assumed to be 2 cm, and the immobile water content for case C was set at  $0.05 \text{ cm}^3 \text{ cm}^{-3}$ , with no transfer of solute between the mobile and immobile regions.

#### 4.2. Dual-porosity models

Dual-porosity models assume that water flow is restricted to the fractures (or inter-aggregate pores and macropores), and that water in the matrix (intra-aggregate pores or the rock matrix) does not move at all. Thus, intra-aggregate pores represent immobile pockets that can exchange, retain and store water, but do not permit convective flow. This conceptualization leads to two-region, dual-porosity type flow and transport models (Phillip, 1968; van Genuchten and Wierenga, 1976) that partition the liquid phase into mobile (flowing, inter-aggregate),  $\theta_f$ , and immobile (stagnant, intra-aggregate),  $\theta_m$ , regions:

$$\theta = \theta_f + \theta_m \quad (8)$$

with some exchange of water and/or solutes possible between the two regions, usually calculated by means of a first-order process. We will use here the subscript  $f$  to represent fractures, inter-aggregate pores, or

macropores, and the subscript  $m$  to represent the soil matrix, intra-aggregate pores, or the rock matrix.

The dual-porosity formulation for water flow can be based on a mixed formulation of the Richards equation (1) to describe water flow in the fractures and a mass balance equation to describe moisture dynamics in the matrix as follows:

$$\frac{\partial \theta_f}{\partial t} = \frac{\partial}{\partial z} \left[ K(h) \left( \frac{\partial h}{\partial z} + 1 \right) \right] - S_f - \Gamma_w, \quad (9)$$

$$\frac{\partial \theta_m}{\partial t} = -S_m + \Gamma_w$$

where  $S_f$  and  $S_m$  are sink terms for both regions, and  $\Gamma_w$  is the transfer rate for water from the inter- to the intra-aggregate pores.

An alternative approach for flow in the macropores was suggested by Germann (1985) and Germann and Beven (1985). They used a kinematic wave equation to describe gravitational movement of water in macropores as follows:

$$\frac{\partial q}{\partial t} + C \frac{\partial q}{\partial z} + cr\theta_f = 0 \quad (10)$$

where  $r$  is the macropore sorbance, and where the volumetric flux density,  $q$ , and the kinematic wave velocity,  $C$ , are defined by:

$$q = b\theta_f^a \quad (11)$$

$$C = \frac{\partial q}{\partial \theta_f} \quad (12)$$

in which  $a$  is a kinematic exponent and  $b$  a macropore conductance parameter. One advantage of this approach is that no water retention properties of the macropore region are required, and hence that the number of parameters can be reduced. Such data are experimentally very difficult to determine. One disadvantage is that the kinematic wave equation is limited to vertical gravity-driven flow, since capillarity is ignored. Thus, application to two-dimensional flow problems (i.e. lateral or downslope flows) faces some numerical and conceptual problems. The kinematic wave approach also cannot explain the non-equilibrium upward infiltration reported by Šimůnek et al. (2001). Contrary to kinematic wave models, dual-porosity models based on the Richards equation do account for both gravitational flow and capillary-driven flow. Hence, Eq. (9) can describe not

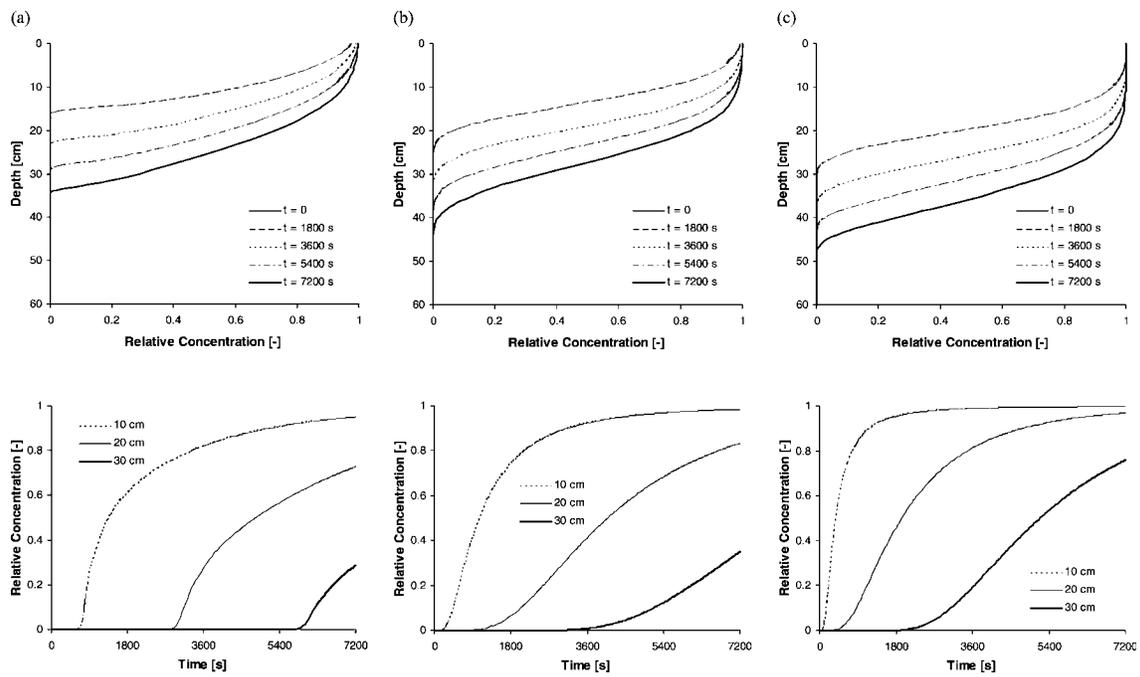


Fig. 3. Concentration profiles (top) and breakthrough curves at 10, 20, and 30 cm (bottom) calculated assuming (a) equilibrium water flow (Eq. (1)) and solute transport (Eq. (2)), (b) non-equilibrium water flow (Eq. (7)) (Ross and Smettem, 2000) and equilibrium solute transport (Eq. (2)), and (c) both non-equilibrium water flow (Eq. (7)) and non-equilibrium solute transport (Eq. (13)).

only vertical downward flow during sudden rainfall events, but also upward flow during evaporation periods.

The dual-porosity formulation for solute transport is similarly based on the convection–dispersion and mass balance equations as follows

$$\begin{aligned} \frac{\partial \theta_f c_f}{\partial t} + \frac{\partial f \rho_s c_f}{\partial t} &= \frac{\partial}{\partial z} \left( \theta_f D_f \frac{\partial c_f}{\partial z} \right) - \frac{\partial q c_f}{\partial z} - \phi_f - \Gamma_s, \\ \frac{\partial \theta_m c_m}{\partial t} + \frac{\partial (1-f) \rho_s c_m}{\partial t} & \\ &= -\phi_m + \Gamma_s \end{aligned} \quad (13)$$

for the fractures (macropores) and matrix, respectively, where  $f$  is the dimensionless fraction of sorption sites in contact with the fractures (mobile water), and  $\Gamma_s$  is the solute transfer rate between the two regions. Although dual-porosity models have been popularly used for solute transport studies (van Genuchten, 1981), their application to water flow problems has been attempted far less frequently.

As an example, Fig. 4 shows computed water and solute distributions during infiltration obtained with a dual-porosity model. The soil hydraulic parameters of the macropore domain were taken as follows:  $\theta_r = 0.0$ ,  $\theta_s = 0.200$ ,  $\alpha_1 = 0.041 \text{ cm}^{-1}$ ,  $n = 1.964$ ,  $l = 0.5$ ,  $K_s = 0.000722 \text{ cm s}^{-1}$ , while the immobile matrix domain was assumed to have a saturated water content,  $\theta_{sm}$ , of 0.15. Initial conditions were set equal to the pressure head of  $-150 \text{ cm}$ . We assumed that water mass transfer was described with Eq. (20), in which the mass transfer constant  $\omega$  was set at  $0.00001 \text{ s}^{-1}$ . For simplicity, we considered only convective solute mass transfer between the two pore regions (i.e. no diffusive transfer), with the dispersivity again fixed at 2 cm. While for ponded surface conditions water in the fracture domain quickly reached full saturation (Fig. 4(a)), the water content of the matrix increased only gradually with time. Consequently, the total water content, defined as the sum of water contents in both the fracture and matrix domains, also increased only gradually. The total water content would be the quantity measured with most field water content measurement devices, such as TDR or neutron probe. Pressure head measurements using tensiometers are on the other hand, often dominated by the wetter fracture domain that reaches equilibrium relatively quickly. Similarly

to the model of Ross and Smettem (2000), as well as other more complex non-equilibrium models, the dual-porosity model can therefore explain often observed non-equilibrium between pressure heads and water contents (Šimůnek et al., 1999b, 2001, among others). Similar non-equilibrium profiles as for the water content were also obtained for the solute concentration (Fig. 4(b)).

#### 4.3. Dual-permeability models

Different types of dual-permeability approaches may be used to describe flow and transport in structured media. Several assume similar governing equations to describe flow in the fracture and matrix regions, while others use different formulations for the two regions. A typical example of the first approach is the work of Gerke and van Genuchten (1993a, 1996) who applied Richards equations to each of two pore regions. The flow equations for the fracture (subscript f) and matrix (subscript m) pore systems are, respectively,

$$\frac{\partial \theta_f}{\partial t} = \frac{\partial}{\partial z} \left( K_f \frac{\partial h_f}{\partial z} + K_f \right) - S_f - \frac{\Gamma_w}{w} \quad (14)$$

and

$$\frac{\partial \theta_m}{\partial t} = \frac{\partial}{\partial z} \left( K_m \frac{\partial h_m}{\partial z} + K_m \right) - S_m + \frac{\Gamma_w}{1-w} \quad (15)$$

where  $w$  is the ratio of the volumes of the fracture (inter-aggregate) and the total pore systems,  $\theta_{fs}/\theta_s$ . This approach is relatively complicated in that the model requires characterization of water retention and hydraulic conductivity functions (potentially of different form) for both pore regions, as well as the hydraulic conductivity function of the fracture–matrix interface (to be discussed later). Note that the water contents  $\theta_f$  and  $\theta_m$  in Eqs. (14) and (15) have different meanings than in Eq. (7) where they represented absolute value of the water content in the total pore-space, while here they denote water contents in the pore-subspace (fracture or matrix).

A similar expression to Eq. (11) for the volumetric flux density in macropores,  $q$ , was suggested by Jarvis (1994) for use in the dual-permeability model

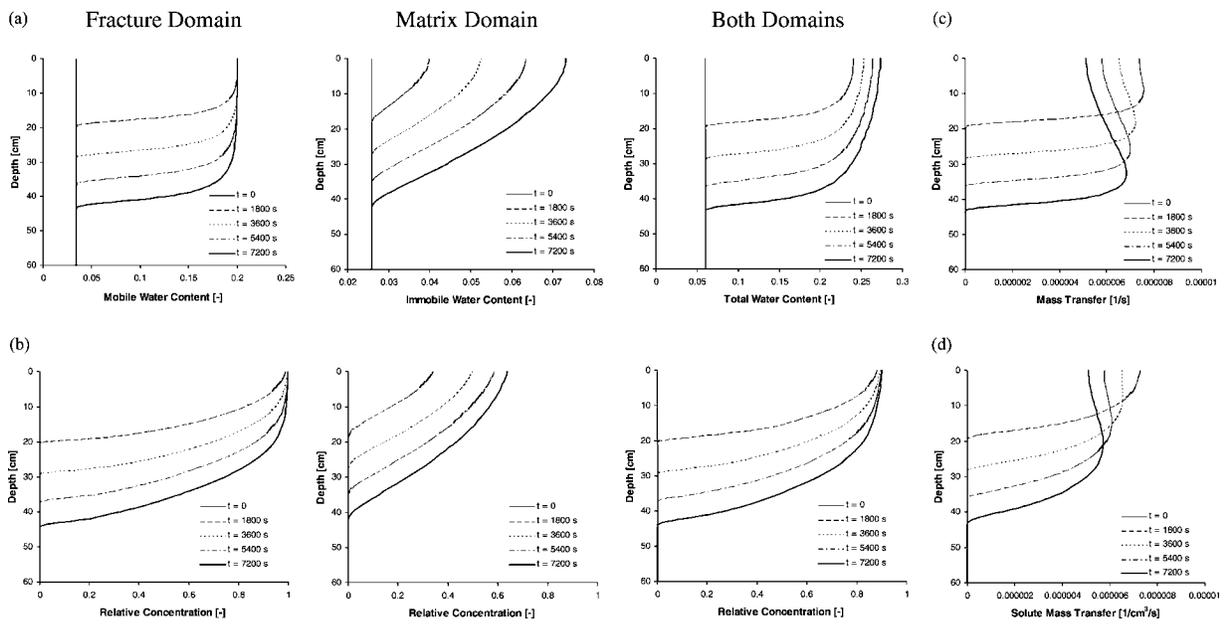


Fig. 4. Water content (a) and concentration (b) profiles in the fracture domain, matrix domain, and both domains combined, as well as water (c) (Eq. (20)) and solute (d) (Eq. (27)) mass transfer terms calculated with the dual-porosity model.

MACRO:

$$q = b \left( \frac{\theta_f}{\theta_{sf}} \right)^a = b(S_e^f)^a \quad (16)$$

where  $\theta_{sf}$  is the saturated water content of the macropores (i.e. macroporosity). Since the macropore water content in Eq. (16) is scaled by  $\theta_{sf}$ , the fracture conductance parameter,  $b$ , has the more direct physical meaning of the hydraulic conductivity of macropores at full saturation. We note that the MACRO model assumes applicability of the Richards equation to flow in the soil matrix.

An alternative approach for flow in the matrix and fractures was used by Ahuja and Hebson (1992) in the RZWQM model. They described infiltration and redistribution in the soil matrix with the Green–Ampt and Richards equations, respectively, and infiltration into cylindrical macropores using Poiseuille’s law assuming gravitational flow:

$$q = \frac{N_p \rho g \pi r_p^4}{8\nu} \quad (17)$$

where  $N_p$  is the number of pores per unit area,  $\rho$  is the density of water,  $g$  is the gravitational constant,  $r_p$  is the radius of the macropores, and  $\nu$  the dynamic viscosity of water. Ahuja and Hebson (1992) used a similar Poiseuille-type expression for planar fractures. One disadvantage of using pore-scale physical laws is that macropores probably rarely flow at full saturation, while their shape, form and continuity will not normally correspond to the assumed simplified geometry.

Analogous to Eqs. (14) and (15), the dual-permeability formulation for solute transport can be based on convection–dispersion type equations for transport in both the fracture and matrix regions as follows (Gerke and van Genuchten, 1993a):

$$\begin{aligned} \frac{\partial \theta_f c_f}{\partial t} + \frac{\partial f \rho s_f}{\partial t} \\ = \frac{\partial}{\partial z} \left( \theta_f D_f \frac{\partial c_f}{\partial z} \right) - \frac{\partial q c_f}{\partial z} - \phi_f - \frac{\Gamma_s}{w} \end{aligned} \quad (18)$$

$$\begin{aligned} \frac{\partial \theta_m c_m}{\partial t} + \frac{\partial (1-f) \rho s_m}{\partial t} \\ = \frac{\partial}{\partial z} \left( \theta_m D_m \frac{\partial c_m}{\partial z} \right) - \frac{\partial q c_m}{\partial z} - \phi_m - \frac{\Gamma_s}{1-w} \end{aligned} \quad (19)$$

Eq. (18) assumes a complete convective–dispersive type transport description for the fractures. Several authors simplified transport in the macropore domain, for example, by considering only piston displacement of solutes (Ahuja and Hebson, 1992; Jarvis, 1994).

Fig. 5 shows an application of the dual-permeability model of Gerke and van Genuchten (1993a) to infiltration into a macroporous soil profile. We used the following soil hydraulic parameters for the matrix ( $\theta_r = 0.105$ ,  $\theta_s = 0.50$ ,  $\alpha_1 = 0.005 \text{ cm}^{-1}$ ,  $n = 1.5$ ,  $l = 0.5$ ,  $K_s = 1.05 \text{ cm d}^{-1}$ ), the fracture ( $\theta_r = 0.0$ ,  $\theta_s = 0.50$ ,  $\alpha_1 = 0.1 \text{ cm}^{-1}$ ,  $n = 2.0$ ,  $l = 0.5$ ,  $K_s = 2000.0 \text{ cm d}^{-1}$ ), and the matrix–fracture interface ( $w = 0.05$ ,  $\beta = 3$ ,  $\gamma = 0.4$ ,  $a = 1.0$ , and  $K_{as} = 0.01 \text{ cm d}^{-1}$ , see Eq. (24)) domains. We assumed that water mass transfer was described with Eq. (23). Similarly as for the dual-porosity example, we again considered only convective solute mass transfer between the two pore regions, with a dispersivity of 2 cm. The initial pressure head for both regions was equal to  $-100 \text{ cm}$ , while water was applied only to the soil matrix until ponding occurred. The soil matrix at the surface quickly became saturated since the applied water flux ( $50.0 \text{ cm d}^{-1}$ ) greatly exceeded the saturated hydraulic conductivity of the matrix ( $K_s = 1.05 \text{ cm d}^{-1}$ ) (Fig. 5(a)). Water started to flow into the fracture domain (Fig. 5(b)) where it moved vertically downwards (Fig. 5(c)) and infiltrated into the matrix domain (Fig. 5(d)). The two distinct moisture fronts in Fig. 5(b) (and concentration fronts in Fig. 5(e)) are due to lateral transfer from the fracture domain (the leading edge), and flow in the matrix domain (the second front). Again, in order to demonstrate sensitivity of the model predictions to the mass transfer coefficient (see Eq. (24)), we included into Fig. 5 final profiles ( $t = 0.08 \text{ d}$ ) calculated when the conductivity of the matrix–fracture interface was decreased or increased by 25% (i.e.  $K_{as} = 0.0075$  and  $0.0125 \text{ cm d}^{-1}$ , respectively).

#### 4.4. Fine-textured soils

Another class of models has been developed for fine-textured swelling clay soils containing shrinkage cracks. Models of this type may take into account shrinking and swelling as a function of the water content, and use statistical properties of cracks (e.g. depth and width) as parameter input. Thus, they do not

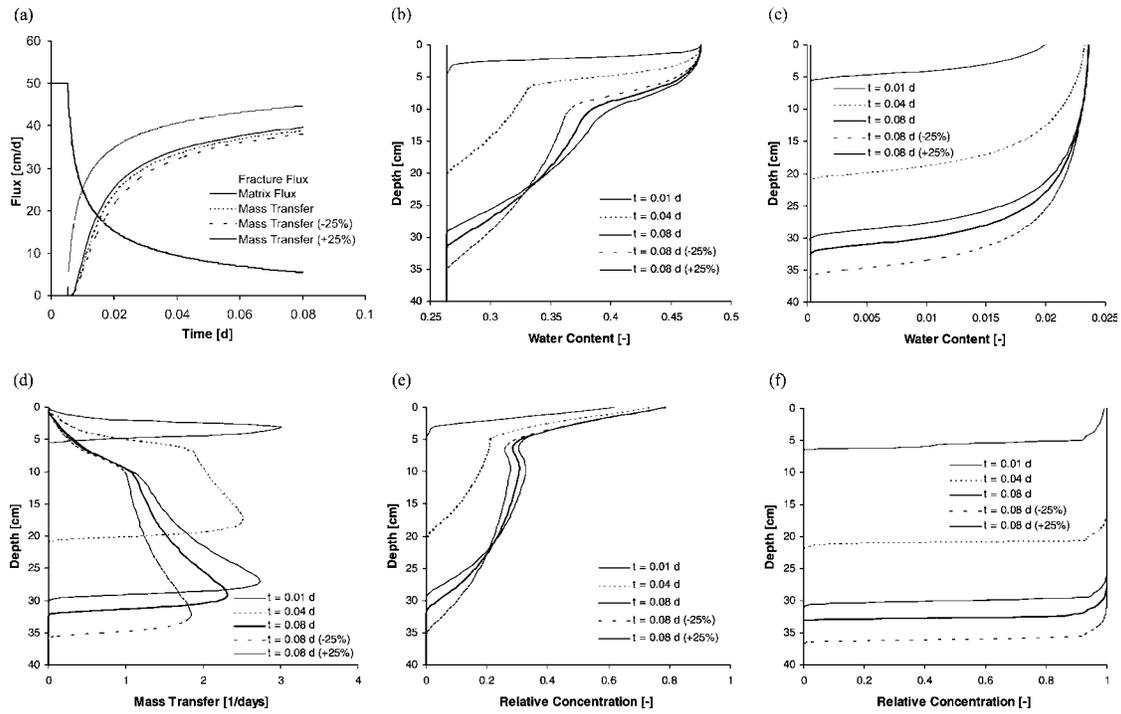


Fig. 5. Infiltration and mass exchange fluxes (a), water contents in the matrix (b) and fracture (c) domains, water mass exchange rates (d) and concentrations in the matrix (e) and fracture (f) domains calculated with the dual-permeability model of Gerke and van Genuchten (1993a,b). Thin lines represent final profiles ( $t = 0.08$  d) when the conductivity of the interface is decreased or increased by 25%.

require detailed knowledge of the crack system and/or the spatial distribution of macropores (Slawinski et al., 1996; van Dam et al., 1997). These models typically assume that water and solutes can move instantaneously to specified bypass depths once the infiltration capacity of the soil matrix is exceeded by the rainfall rate and a critical depth of water has formed at the soil surface (Verburg et al., 1996; van Dam et al., 1997; Novák et al., 2000). Downward bypassing or short-circuiting will not occur if the matrix absorbs all water through the soil surface. Since in all of these models water flow in the matrix is described using the Richards equation, while water in the cracks moves from the soil surface to some specified depth (albeit instantaneously), these models can be viewed as a subgroup of the dual-permeability models. Water infiltrating from the cracks into the soil matrix is estimated using either Darcy's law (van Dam et al., 1997) or the Green–Ampt approach (Novák et al., 2000) and then added as a source term to the Richards equation describing flow in the soil matrix.

Fig. 6 compares various fluxes for two infiltration scenarios, one with and one without the presence of soil drying cracks as calculated with the fracture program of Novák et al. (2000). Because the applied water flux ( $25 \text{ cm d}^{-1}$  for 2 h) at the soil surface (curve 1) is much higher than the saturated hydraulic

conductivity of the matrix ( $K_s = 5 \text{ cm d}^{-1}$ ), the soil surface ponds quickly, a critical layer of water forms on the soil surface, and water either further accumulates at the soil surface or starts to run off when no cracks are present. Alternatively, when cracks are present, water starts to flow into the cracks (curve 5), from which it infiltrates into the soil (curve 4). As expected, when water is allowed to accumulate on the soil surface (no cracks present; curve 2), it takes much longer for this water to infiltrate than when it is allowed to flow into cracks (curve 3). If water is not allowed to accumulate on the soil surface and no cracks are present (curve 3), then most of this water is lost by surface run off (curve 5). When cracks are present, cumulative infiltration (curve 6) proceeds much faster than when water is allowed to accumulate at the soil surface (curve 2), and is much larger than when water is allowed to run off (curve 3). We refer to Novák et al. (2000) for a more detailed discussion of this example.

#### 4.5. Multiple-porosity/permeability models

Multiple-porosity/permeability models are conceptually similar to dual-porosity/permeability models, except that they implement additional overlapping pore regions. This allows for greater flexibility, albeit

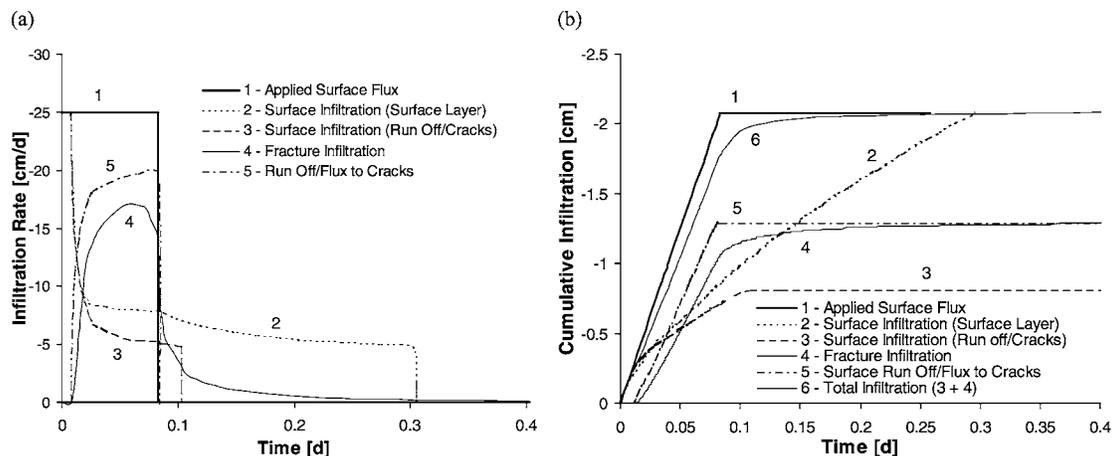


Fig. 6. Actual (a) and cumulative (b) fluxes versus time for infiltration of water into a soil with and without cracks and/or macropores (after Novák et al. (2000)): (1) irrigation, (2) infiltration into a soil without cracks with water accumulating on the soil surface, (3) infiltration through the soil surface with surface runoff or with cracks present, (4) infiltration from the cracks into the soil matrix, (5) flow into cracks or surface run off, and (6) total infiltration into the soil matrix when cracks are present.

at the expense of requiring more parameters that may also be physically poorly defined. For example, Gwo et al. (1995) developed the MURF and MURT models for multi-region flow and transport, respectively, assuming three overlapping pore regions: macropores, mesopores, and micropores (or using alternative terms: primary fractures, secondary fractures and soil matrix). Although different functions for the soil hydraulic properties of each region were used, they assumed applicability of the Richards and convection–dispersion equations in all three regions. Hutson and Wagenet (1995) developed the TRANSMIT model that considers  $n$  overlapping regions, with flow and transport in each region again described using the Richards and convection–dispersion equations. Similar to Gwo et al. (1995), they allowed for water and solute to exchange between all regions.

#### 4.6. Functional approaches

A large number of functional models, generally capacity type approaches, has also been developed to account for preferential water flow and/or solute transport (Addiscott, 1977; Addiscott et al., 1986; Corwin et al., 1991; Emermann, 1995). These approaches are usually motivated by a desire to work with relatively simple preferential models that require only a few parameters. One disadvantage inherent to these functional models is that the rate of macropore flow may depend implicitly on the adopted time step in the model. Emermann (1995) showed that a simple tipping bucket model for macropore flow could be reformulated in terms of a differential equation, thereby avoiding this limitation. The resulting model resembles the kinematic wave equation discussed earlier, with the difference that Emermann (1995) assumed that macropore flow was a linear function of the macropore water content.

### 5. Mass transfer

Critical in all dual-porosity/permeability models are the coupling terms  $\Gamma_w$  and  $\Gamma_s$  describing mass transfer between the fracture and matrix regions. Some descriptions are physically based, though approximate, while others are entirely empirical.

Below we list some of the formulations most often used.

#### 5.1. Mass transfer driven by fluid saturation

The mass transfer rate,  $\Gamma_w$ , for water between the fracture and matrix regions in several dual-porosity studies (Phillip, 1968; Šimůnek et al., 2001) has been assumed to be proportional to the difference in effective water contents of the two regions using the first-order rate equation:

$$\Gamma_w = \frac{\partial \theta_m}{\partial t} = \omega[S_e^f - S_e^m] \quad (20)$$

where  $\theta_m$  is the matrix water content,  $\omega$  is a first-order rate coefficient ( $T^{-1}$ ), and  $S_e^f$  and  $S_e^m$  are effective fluid saturations of the fracture and matrix regions, respectively. Compared to assuming a pressure head-based driving force (to be discussed later), the dual-porosity model based on this mass transfer equation requires significantly fewer parameters since one does not need to know the retention function for the matrix region explicitly, but only its residual and saturated water contents. Coupling (Eq. (20)) with a dual-porosity non-equilibrium flow model leads to the usual soil hydraulic parameters needed for the equilibrium model, two additional parameters characterizing the matrix region (i.e. its residual,  $\theta_r^m$ , and saturated,  $\theta_s^m$ , water contents), and the first-order mass transfer coefficient  $\omega$ . By additionally assuming that the residual water content of the fracture region is equal to zero (and hence that residual water is present only in the immobile region), one could further decrease the number of model parameters. The resulting model was used for the calculations shown in Fig. 3.

Eq. (20) assumes that the mass transfer rate is proportional to the difference in effective water contents, rather than pressure heads (Gerke and van Genuchten, 1993b), which should provide a more realistic description of the exchange rate between the fracture and matrix regions. Eq. (20) thus inherently assumes that the water retention properties of the matrix and the fracture domains are identical. For this reason, Eq. (20) must be used with some caution and probably only for dual-porosity models. Dual-porosity models that use Eq. (20) are in some respects conceptually similar to the non-equilibrium

model of Ross and Smettem (2000) discussed earlier. This is because both models assume that the approach to equilibrium (as characterized by either the mass transfer coefficient  $\omega$  or the equilibration time constant  $\tau$ ) is independent of the actual saturation level, only to its absolute deviation from equilibrium.

In the absence of gravity, the Richards equation can be recast for a homogeneous medium as a diffusion equation with gradients in water content as the driving force. The dual-permeability model MACRO (Jarvis, 1994) uses a formulation for the mass transfer term that is based on a first-order approximation to the water diffusion equation:

$$\Gamma_w = \frac{\partial \theta_m}{\partial t} = \left( \frac{\beta D_w \gamma_w}{d^2} \right) (\theta_b - \theta_m) \quad (21)$$

where  $\theta_b$  is the saturated water content in micropores,  $d$  is an effective ‘diffusion’ pathlength (i.e. half the aggregate width or half the fracture spacing),  $\beta$  is a shape factor that depends on the geometry, and  $\gamma_w$  is a scaling factor (= 0.4) obtained by matching the results of the first-order approach at the half-time level of the cumulative infiltration curve to the numerical solution of the horizontal infiltration equation (Gerke and van Genuchten, 1993b). The effective water diffusivity  $D_w$  given by

$$D_w = \left( \frac{D_{\theta_b} + D_{\theta_m}}{2} \right) S_e^f \quad (22)$$

where  $D_{\theta_b}$  and  $D_{\theta_m}$  are soil water diffusivities at saturation (saturation is assumed to exist at the fracture–matrix interface,  $\theta_b$ ) and in the matrix ( $\theta_m$ ), respectively, and where the effective saturation of the macropores,  $S_e^f$ , is introduced to account for an incomplete wetted contact area between the two pore domains. The value of  $\beta$  varies with the geometry assumed for the aggregates (van Genuchten and Dalton, 1986) and in MACRO this parameter is set to 3 for rectangular slabs. The model based on Eqs. (21) and (22) is clearly more physically based than Eq. (20) since the water content driving force pertains to the same material (i.e. the matrix), being given by the difference between the saturated water content of the micropores (i.e. the water content at the interface between micropores and macropores when macropores are active) and the average water content of the micropores. It is therefore assumed that during active water exchange between micropores and macropores,

the water pressures at the interface instantaneously reach equilibrium at the water-entry pressure of the macropores. It can be noted that this is not the same as assuming that the matrix has to be saturated for bypass flow of water to occur in the macropores. Eq. (21) only describes flow from macropores to matrix and not in the reverse direction. It is intended for use in models based on cut and join hydraulic functions (i.e. similar to Eq. (5)) and could not be used without modification in dual-permeability models based on the concept of overlapping pore continua (i.e. Eqs. (3) and (4)). In MACRO, the boundary between macropores and matrix is defined by the saturated matrix water content (defined earlier), the equivalent pressure head ( $h_b$ ) and the hydraulic conductivity at  $\theta_b$  and  $h_b$  (Jarvis, 1994). Flow from matrix to macropores occurs instantaneously if the matrix water content exceeds  $\theta_b$  (i.e. the matrix pressure head exceeds  $h_b$ ), following the basic physical principle that governs the filling of pores when the water-entry pressure is exceeded. This can occur internally within the soil, and also at the soil surface when rainfall intensity exceeds the matrix infiltration capacity.

## 5.2. Mass transfer driven by pressure head gradient

The rate of exchange of water between the fracture and matrix regions,  $\Gamma_w$ , can also be assumed to be proportional to the difference in pressure heads between the two pore regions (Gerke and van Genuchten, 1993a):

$$\Gamma_w = \alpha_w (h_f - h_m) \quad (23)$$

in which  $\alpha_w$  is a first-order mass transfer coefficient. Since pressure heads are now needed for both regions, this approach requires estimating retention curves for both pore regions. For porous media with well-defined geometries, the first-order mass transfer coefficient,  $\alpha_w$ , can be defined as follows (Gerke and van Genuchten, 1993b):

$$\alpha_w = \frac{\beta}{d^2} K_a \gamma_w \quad (24)$$

Gerke and van Genuchten (1996) evaluated the effective hydraulic conductivity  $K_a$  of the fracture–matrix interface using a simple arithmetic average

involving both  $h_f$  and  $h_m$  as follows

$$K_a(h) = 0.5[K_a(h_f) + K_a(h_m)] \quad (25)$$

The use of Eq. (24) implies that the medium contains geometrically well-defined rectangular or other types of macropores or fractures (Edwards et al., 1979; van Genuchten and Dalton, 1986). While geometrically based models are conceptually attractive, they may be too difficult to use for field applications, partly because structured soils and rocks usually contain mixtures of aggregates and matrix blocks of various sizes and shapes, but also because the parameters in Eq. (24) may not be identifiable. Hence, rather than using Eq. (24) directly, one could also lump  $\beta$ ,  $d$ , and  $\gamma_w$  into one effective hydraulic conductivity  $K_a^*$  of the fracture–matrix interface to give

$$\alpha_w = K_a^*(h) \quad (26)$$

in which case  $K_a^*$  can then be used as calibration parameter. To overcome the requirement for geometrically well-defined macropores or fractures in Eq. (24), Gerke and van Genuchten (1996) suggested a method for deriving values of the shape factor  $\beta$  in Eq. (24) for non-idealized geometries or mixtures of shapes in order to obtain a more general ‘macroscopic’ approach.

Because one needs to define retention curves for both regions, mass transfer based on pressure head differences is more complex than mass transfer based on a water content difference. Nevertheless, it may be preferred to Eq. (20) since the difference in pressure heads is the actual driving force for mass transfer. On the other hand, the mass transfer term given by Eq. (23) may be inherently more unstable numerically since it involves calculating the product of two highly non-linear terms, each of which can become extremely small or large. In contrast, Eq. (21) is more stable since the diffusivity term is less non-linear than  $K$ , while the water content differences never become extreme. Mass transfer based on Eqs. (23) and (24) was used for the calculations presented in Fig. 5.

In order to demonstrate the difficulty in distinguishing between various dual-porosity/permeability models and between various descriptions of mass transfer, which is practically very difficult, if not impossible, to measure, we repeated the calculations presented in Fig. 4 using different definitions for the mass transfer term with all other parameters, initial

and boundary conditions the same as before. Fig. 7 shows distributions versus depth of the water mass exchange rate,  $\Gamma_w$ , calculated with the dual-porosity model when using the saturation driven exchange term (Eq. (20)) and the pressure head driven exchange term (Eq. (23)) assuming a constant (independent of  $h$ ) and variable (dependent on  $h$ ) parameter  $\alpha_w$  (Eq. (24)). The soil hydraulic parameters for the matrix, for the pressure head driven case, were taken to be the same as for the fracture domain. The first-order rate coefficients  $\omega$  and  $\alpha_w$  in the saturation and pressure head driven (assuming a constant parameter  $\alpha_w$ ) mass transfer terms were set equal to  $1.0 \times 10^{-5} \text{ s}^{-1}$  and  $1.0 \times 10^{-7} \text{ cm}^{-1} \text{ s}^{-1}$ , respectively. The parameter  $K_{as}^*$  in the pressure head driven mass transfer with a variable parameter  $\alpha_w$  was set equal to  $4.0 \times 10^{-7} \text{ cm}^{-1} \text{ s}^{-1}$ . Although radically different descriptions of the mass transfer term were used in these calculations, all three runs resulted into visually almost identical pressure head and water content profiles in the fracture domain, while only very small differences were noticeable in the matrix domain (Fig. 4). Fig. 7 reflects different levels of non-linearity in the various definitions of the mass transfer term. While effective saturation can range between 0 and 1, pressure heads in these calculations ranged between  $-150 \text{ cm}$  and 0. This is the main reason why the first-order rate coefficients in the saturation and pressure head driven mass transfer terms vary by a factor of up to two.

### 5.3. Other approaches to mass transfer

Several other approaches for calculating the mass transfer term have also been used. For example, Ahuja and Hebson (1992) and Novák et al. (2000) modeled mass transfer using the Green and Ampt equation, Chen and Wagenet (1992) used the Philip infiltration model, while Zimmerman et al. (1993) used the Warren–Root model, as well as developed their own formulation.

### 5.4. Solute mass transfer

The transfer rate,  $\Gamma_s$ , for solutes between the fracture and matrix regions is usually given as the sum of diffusive and convective fluxes, and can be written

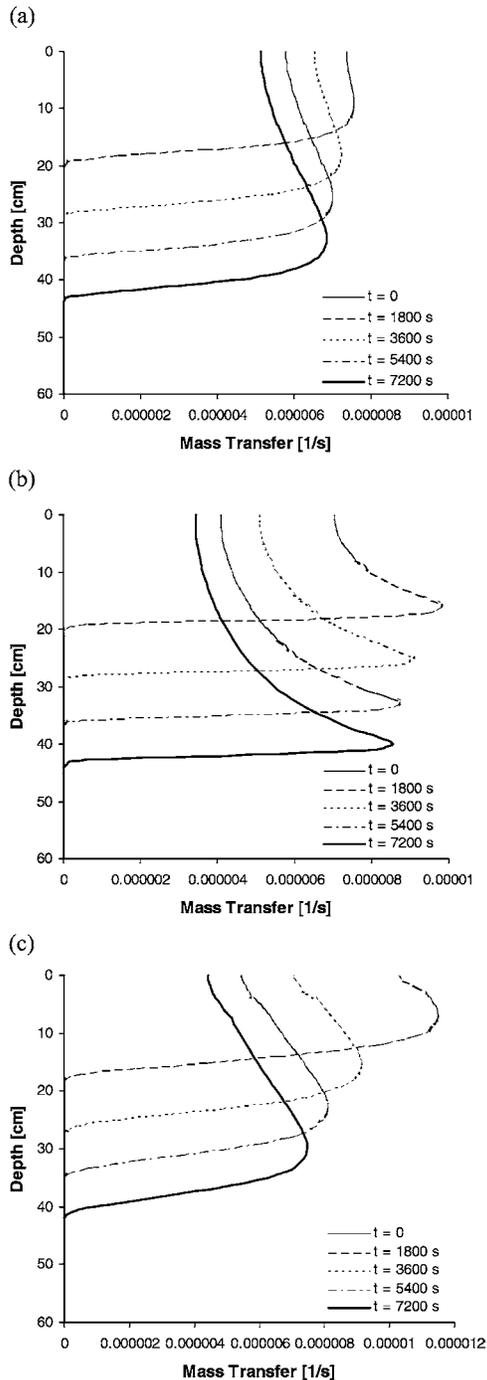


Fig. 7. The water mass exchange rate profiles calculated with the dual-porosity model with (a) the saturation driven exchange term (Eq. (20)), and the pressure head driven exchange term (Eq. (23)) with (b) a constant and (c) variable parameter  $\alpha_w$  (Eq. (24)).

as (Gerke and van Genuchten, 1996):

$$\Gamma_s = \alpha_s(1 - w_m)(c_f - c_m) + \Gamma_w c^* \quad (27)$$

where  $c^*$  is equal to  $c_f$  for  $\Gamma_w > 0$  and  $c_m$  for  $\Gamma_w < 0$ , and  $\alpha_s$  is the first-order solute mass transfer coefficient ( $T^{-1}$ ) of the form

$$\alpha_s = \frac{\beta}{d^2} D_a \quad (28)$$

in which  $D_a$  is an effective diffusion coefficient ( $L^2 T^{-1}$ ) which represents the diffusion properties of the fracture–matrix interface, as well as other parameters.

## 6. Model complexity and parameterization

The main disadvantage of dual-porosity and dual-permeability models is that, contrary to models for a single pore region, they require many more input parameters to characterize both pore systems. For example, the dual-permeability model of Gerke and van Genuchten (1993a), in its full complexity, needs 16 parameters to describe water flow. This is because the hydraulic properties of the fracture and matrix regions are each characterized by six soil hydraulic parameters (the same number as the equilibrium system). Additionally, estimates of structural parameter  $w$ , as well as  $K_{as}^*$ ,  $\alpha_a$ , and  $n_a$  are needed to characterize the hydraulic conductivity of the fracture–matrix interface when using the Mualem–van Genuchten model. A previous assumption (Gerke and van Genuchten, 1993a, 1996) is that the relative hydraulic conductivity functions of the interface and the matrix regions are the same, thus requiring only the saturated interface conductivity  $K_{as}^*$  to scale the interface relative hydraulic conductivity function. If the pore connectivity parameters,  $l$ , are equal to 0.5 (Mualem, 1976) and, as before, the residual water content of the mobile region is assumed to be zero, the number of parameters decreases to eleven:  $w$ ,  $\theta_s^f$ ,  $\theta_r^m$ ,  $\theta_s^m$ ,  $\alpha_f$ ,  $\alpha_m$ ,  $n_f$ ,  $n_m$ ,  $K_s^f$ ,  $K_s^m$  and  $K_{as}^*$ .

The number of input parameters decreases slightly when the kinematic wave approach is used to describe flow in the fracture domain. In this case, the matrix domain is again characterized by six parameters (assuming the Mualem–van Genuchten model), while

the fracture domain and the inter-domain interface are characterized by the macroporosity,  $\theta_{sf}$ , the fracture conductivity,  $b$ , the exponent  $a$ , and an effective diffusion path length  $d$ . Thus, this model needs a total of 10 parameters to describe the porous medium.

A similar number of parameters (i.e. 11) is needed for the dual-porosity model based on the Richards equation, the van Genuchten–Mualem model for the soil hydraulic properties, and the pressure head-based mass transfer term. In this case, one needs six parameters to characterize the fracture domain ( $\theta_r$ ,  $\theta_s$ ,  $\alpha$ ,  $n$ ,  $l$ ,  $K_s$ ), four parameters for the matrix domain ( $\theta_r$ ,  $\theta_s$ ,  $\alpha$ ,  $n$ ), and one parameter for the interface ( $K_{as}^*$ ) (assuming that several other factors can be lumped into this parameter). As discussed earlier, the number of parameters decreases to 9 when the pressure head-based mass transfer term is replaced with the water content-based mass transfer term, since then only the parameters  $\theta_r$  and  $\theta_s$  are needed to characterize the matrix.

The number of parameters of course increases significantly for multi-porosity and multi-permeability models for which one needs to determine or calibrate the soil hydraulic (retention and hydraulic conductivity) parameters for each transport domain, as well as mass transfer coefficients between all transport domains. In contrast, the non-equilibrium model of Ross and Smettem (2000) requires only one additional parameter as compared to equilibrium flow models.

Little guidance is available as to how to obtain these parameters, either by direct measurement, a priori estimation, or some calibration technique (Beven, 1991; Clothier et al., 1995; Jaynes et al., 1995). Existing experiments rarely provide enough information to fully calibrate non-equilibrium flow models, let alone to distinguish between the various non-equilibrium models. As illustrated in Fig. 7, different non-equilibrium models can produce relatively similar results (see also Šimůnek et al. (2001)). Experiments or devices hence must be designed that provide (either directly or by inverse modeling) estimates of the many parameters needed in these relatively complex models. Examples of new approaches for analyzing water transfer properties of aggregates with and without cutans based on tension imbibition have been presented by Leeds-Harrison et al. (1994) and Gerke and Köhne (2002). Disc infiltrimeters can greatly facilitate measurements of

the composite (macropore plus matrix) hydraulic properties. Disc infiltrometry methods involving ponded and tension infiltrimeters are now increasingly used for in situ measurements of the hydraulic conductivity. Advantages of these methods are that they can yield well-defined conductivity functions near saturation, especially when combined with other methods to measure the hydraulic properties at intermediate pressure head values in the mesopore/micropore range (Mohanty et al., 1997; Jarvis et al., 1999). These measurements may also be useful for developing predictive (pedotransfer) functions for model parameters in the absence of data. For example, Smettem and Bristow (1999) showed that hydraulic conductivity measured by tension infiltrimeter at  $-4$  cm in 20 Australian soils was well explained by variation in clay content. On a large dataset for 70 soil horizons from 13 different countries, Jarvis et al. (2002) found weaker but still significant relationships ( $r^2$  values up to 49%) between textural properties and the hydraulic conductivity measured at  $-10$  cm by tension infiltrimeter.

Very little is currently known about the possibilities and potential problems of applying inverse modeling techniques to preferential flow models. Durner et al. (1999) showed that the parameters of bimodal water retention and hydraulic conductivity functions (Eqs. (3) and (4)) could be determined by inverse modeling of multi-step outflow data. They claimed that the procedure was robust, leading to unique solutions with limited data (water flow only), irrespective of the number of parameters included, providing the underlying model accurately represented the true soil hydraulic properties. By comparison, Schwartz et al. (2000) recently attempted to estimate the parameters of a dual-permeability transport model by inverse modeling using steady-state solute breakthrough data from a variably charged tropical soil, in which the bromide ion may behave as a weakly sorbed reactive solute. They encountered great difficulties in obtaining physically realistic estimates of two critical parameters: the dispersion coefficient in the micropores ( $D_m$  in Eq. (19), which became far too large), and the fraction of sorption sites in the macropores ( $f$  in Eqs. (13), (18), and (19)), which tended towards unity (i.e. all sorption sites presumably are located in the macropores).

They concluded that inverse procedures are problematic for dual-permeability transport models, even for the simple case of steady water flow with only four unknown parameters. However, the data set available to Schwartz et al. (2000) was not ideal in that no conservative tracer was applied (bromide was reactive in their soil), while only flux measurements at the base of the column were available, but no resident concentrations inside the column. In contrast, Kätterer et al. (2001) used the inverse modeling package SUFI (Abbaspour et al., 1997) to successfully estimate the parameters of the dual-permeability model MACRO using column breakthrough experiments for multiple non-reactive tracers (deuterium, bromide, and chloride) and two soil indigenous solutes (sulphate and nitrate). Their study made use of both outflow flux concentration data and resident concentrations inside the columns at the end of the experiments.

### 7. Need for inter-code comparison

A relatively large number of models has been developed during the last two decades that consider non-equilibrium flow and transport. While several studies have been carried out to compare various codes describing uniform Darcian flow in the vadose zone (Gee et al., 1999; Ogan et al., 1999; Scanlon et al., 2002), similar comparisons of codes and/or approaches simulating preferential and/or non-equilibrium flow are thus far lacking. This may in large part be due to the fact that most of the preferential flow codes are not readily available, are not easy to use, lack numerical stability, and/or are based on such significantly different descriptions of the underlying flow processes that an effective comparison is neither easy nor straightforward.

To be able to carry out such studies, we developed new versions of the HYDRUS-1D and HYDRUS-2D codes (Šimůnek et al., 1998, 1999a) that include a hierarchical system of various approaches simulating preferential or non-equilibrium flow and transport. Versions 2.0 of both codes could deal only with equilibrium water flow (Eq. (1)), and with equilibrium or non-equilibrium mobile–immobile solute transport (Eqs. (2) and (13)). Recently updated versions

additionally include uniform flow with composite retention and hydraulic conductivity functions (Eqs. (3) and (4)), the single-porosity non-equilibrium model of Ross and Smettem (2000) (Eq. (7)), a dual-porosity model based on the Richards equation (9) with either the water content or the pressure head-based mass transfer terms (Eqs. (20) and (23)), and finally two dual-permeability models: one using the Richards equation for both pore regions (Eqs. (14) and (15)), and one using the kinematic wave approach for flow in the macropores (Eq. (16)). The different examples discussed in this paper were all obtained with the updated HYDRUS-1D code.

### 8. Concluding remarks

While macropore flow has important effects on subsurface hydrology in general, and on infiltration rates and unsaturated soil water distributions in particular, its main implications are likely in the accelerated movement of surface applied fertilizers or pollutants through the vadose zone (Nielsen et al., 1986). At present it is still very difficult to use the more complex dual-permeability model involving two coupled Richards equations to describe preferential flow and transport under field conditions, partly because of the large number of parameters involved, and the current lack of standard experimental techniques to obtain them. At present no examples exist of such applications in the soil science and vadose zone hydrology literature. Hence, the use of these models has so far been restricted to theoretical applications and laboratory studies carried out under well-defined and controlled conditions. The dual-permeability model MACRO, based on the kinematic wave equation for flow in macropores, requires fewer parameters, has been frequently applied to long-term transient field experiments (Villholth and Jensen, 1998; Larsson and Jarvis, 1999a,b) and is also being used for risk assessment for pesticide leaching within the EU (FOCUS, 2000). The main reasons for the wider use of this model are that it is physically based and numerically robust, while the difficult problem of parameterization is not insurmountable.

Accurate coupling of the fracture and matrix domains still represents the greatest challenge in

terms of successfully describing non-equilibrium flow and transport in the vadose zone. Matrix–macropore (or matrix–fracture) interfaces can have very different properties than the bulk matrix due to the deposition of organic matter, various types of coatings, fine-texture mineral particles, or various oxides and hydroxides on the aggregate exteriors or macropore walls; these coatings can markedly reduce rates of diffusion and mass flow between macropores and the soil matrix (Thoma et al., 1992).

With some exceptions (Larsson and Jarvis, 1999a,b), the limited availability of comprehensive data sets has so far restricted the field validation of preferential flow models. A need still remains to apply currently available modeling tools to natural systems where sufficient data are available to first parameterize the models and then to assess the adequacy of model predictions (Šimůnek and de Vos, 1999; Evans et al., 2001). This type of two-stage calibration process (sometimes called historical validation) may be difficult to follow in practice due to experimental difficulties related to inaccessibility and observation scale in fractured rocks or because of the inherently dynamic macropore system in soils being subject to physical (swell/shrink, freeze/thaw), biological (variations in soil faunal activity) and man-made disturbances (ploughing and other tillage practices).

Still, while the problem of modeling preferential flow obviously will remain a challenge, several useful approaches have recently become available to study and model preferential/non-equilibrium flow in structured and/or fractured media. Continuous advances in both numerical techniques and computer hardware are now making it increasingly possible to carry out comprehensive simulations of non-equilibrium flow processes in the vadose zone. Such simulations, especially if paired with good field data sets, are vital to better understanding and quantifying the often-controlling effects of heterogeneities, fractures and macropores on flow and transport at the field scale (van Genuchten et al., 1999).

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