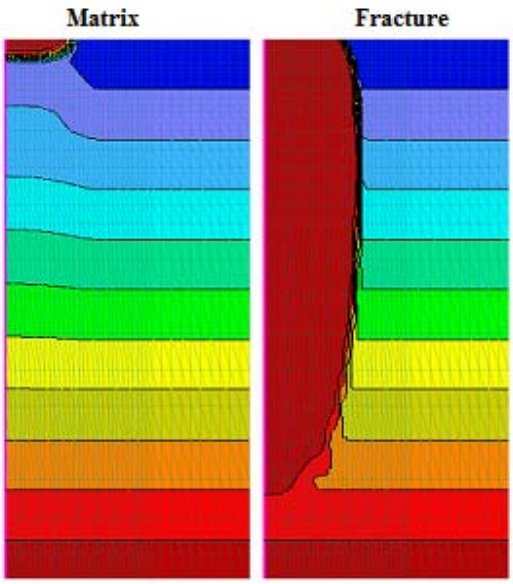
The DualPerm Module

for HYDRUS (2D/3D)

Simulating Two-Dimensional Water Movement and Solute Transport in Dual-Permeability Variably-Saturated Porous Media

Version 1



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Abstract

Šimůnek, J., M. Šejna, and M. Th. van Genuchten, The DualPerm Module for HYDRUS (2D/3D) Simulating Two-Dimensional Water Movement and Solute Transport in Dual-Permeability Porous Media, Version 1.0, PC Progress, Prague, Czech Republic, 32 pp., 2012.

This report documents the **DualPerm** module [*Šimůnek et al.*, 2003; *Šimůnek and van Genuchten*, 2008] for the **HYDRUS (2D/3D)** software package simulating two-dimensional variably-saturated water movement and solute transport in dual-permeability porous media. The dual-permeability flow and transport model assumes that soil consists of two mobile pore regions, one representing the matrix and one the macropores. The dual-permeability formulation for water flow is based on a mixed form of the Richards equation, describing water flow in both the fractures (macropores) and the matrix (micropores) domains [*Gerke and van Genuchten*, 1993a]. The dual-permeability formulation for solute transport is based on a convection-dispersion equation, describing solute transport in both the fractures (macropores) and the matrix (micropores) domains [*Gerke and van Genuchten*, 1993a]. The mass transfer of water between the two domains is driven by the gradient of pressure heads. The mass transfer for solute includes both convective mass transfer with water mass transfer, as well as diffusive mass transfer driven by the concentration gradient. Applications of the **DualPerm** module are demonstrated on several examples. The **DualPerm** module is not intended for large transport domains and should be used preferable for smaller domains.

This report serves as both a **Technical** and **User Manual** and is a reference document of the **Graphical User Interface** of the **DualPerm** related parts of the **HYDRUS** software package.

DISCLAIMER

This report documents the DualPerm module of HYDRUS (2D/3D). The DualPerm module was developed as a supplemental module of the HYDRUS software package, to model the two-dimensional variably-saturated water movement and solute transport in dual-permeability porous media. The software has been verified against selected test cases. However, no warranty is given that the program is completely error-free. If you do encounter problems with the code, find errors, or have suggestions for improvement, please contact one of the authors at

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1. Introduction

There is increasing evidence that flow and transport processes in soils often cannot be described using classical models that assume uniform flow and transport [e.g., *Nkedi-Kizza et al.*, 1984; *Hendrickx and Flury*, 2001; *Pot et al.*, 2005; *Köhne et al.*, 2006]. Many laboratory and field experiments have demonstrated the presence of nonequilibrium flow and transport conditions in soils. Nonequilibrium water flow and solute transport in the unsaturated zone can be simulated at present by means of a large number of models of various degrees of complexity and dimensionality. Modeling approaches range from relatively simple analytical solutions for solute transport [e.g., *van Genuchten*, 1981; *Toride et al.*, 1993] to complex numerical codes [e.g., *Šimůnek et al.*, 2008; *Jacques and Šimůnek*, 2005]. Numerical models are now increasingly being used since they can be applied more readily to realistic laboratory and field problems as compared to analytical models. The use of numerical models has been further popularized during the last 20 years or so because of the appearance of appropriate software packages in both the public and commercial domains, and the development of increasingly sophisticated graphics-based interfaces that can simplify their use tremendously.

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 [*Šimůnek et al.*, 2003; *Šimůnek and van Genuchten*, 2008] (Fig. 1). 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. While the uniform flow model and dual-porosity models are available in the standard version of HYDRUS (2D/3D) (Fig. 1abc), dual-permeability models are not (Fig. 1d).

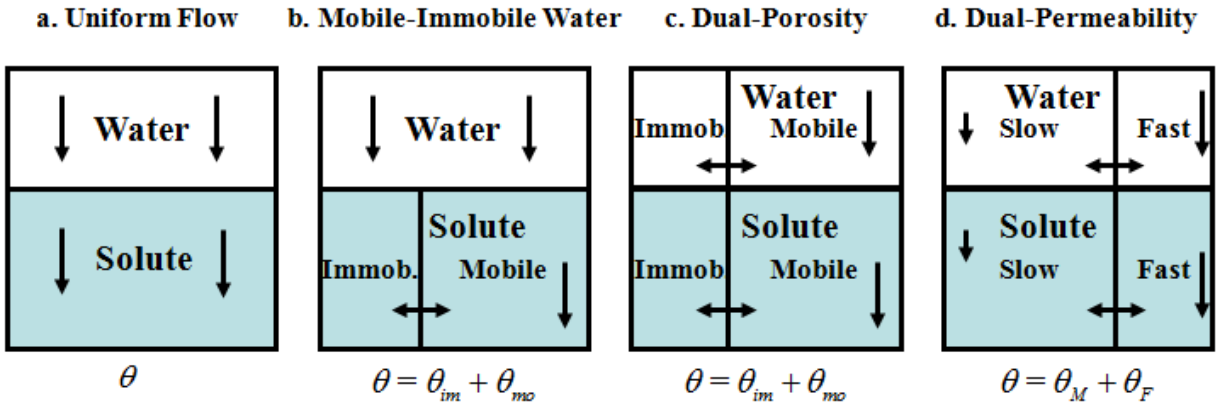

Figure 1. Conceptual physical nonequilibrium models for water flow and solute transport. In the plots, θ is the water content, θ_{mo} and θ_{im} in (b) and (c) are water contents of the mobile and immobile flow regions, respectively; θ_M and θ_F in (d) are water contents of the matrix and macropore (fracture) regions, respectively.

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. Dual-permeability models, in which water can move in both the inter- and intra-aggregate pore regions are now also becoming more popular. 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, the Green and Ampt or Philip infiltration models, the kinematic wave equation, and the Richards equation [*Gerke and van Genuchten*, 1993a].

We have implemented the dual-permeability module **DualPerm** (Fig. 1d) as a supplemental module for HYDRUS (2D/3D) based on the approach suggested by *Gerke and van Genuchten* [1993a]. This report serves as both a Technical and User Manual and is a reference document of the Graphical User Interface of the DualPerm-related parts of the HYDRUS software package simulating two-dimensional variably-saturated water movement and solute transport in dual-permeability porous media. The numerical solution of the two-dimensional variably-saturated water flow, and heat and solute movement are described in the HYDRUS (2D/3D) documentation, and will not be repeated here. The DualPerm module is fully supported by the HYDRUS (2D/3D) graphical user interface [*Šejna et al.*, 2011].

The **DualPerm** module may be used to analyze water and solute movement in unsaturated, partially saturated, or fully saturated porous media. **DualPerm** can handle flow domains delineated by irregular boundaries. The flow region itself may be composed of nonuniform soils having an arbitrary degree of local anisotropy. Flow and transport can occur in the vertical plane, the horizontal plane, or in a three-dimensional region exhibiting radial symmetry about a vertical axis. The water flow part of the model considers prescribed head and flux boundaries, as well as boundaries controlled by atmospheric conditions.

The governing flow and transport equations are solved numerically using standard Galerkin-type linear finite element schemes. Applications of the **DualPerm** module are demonstrated on several examples.

2. Dual-Permeability Water Flow

2.1. *Governing Flow Equations*

Different dual-permeability approaches (Fig. 1) may be used to describe flow and transport in structured media. While some models invoke similar equations for flow in the fracture and matrix regions, others use different formulations for the two regions. A typical example of the first approach, implemented also in HYDRUS-1D, is the work of *Gerke and van Genuchten* [1993ab, 1996] who applied the Richard equation to each of the two pore regions. The flow equations for the macropore (fracture) (subscript *f*) and matrix (subscript *m*) pore systems in their approach are given by

$$\begin{aligned}\frac{\partial \theta_f(h_f)}{\partial t} &= \frac{\partial}{\partial x_i}\left[K_f(h_f)\left(K^A_{ij,f}\frac{\partial h_f}{\partial x_j} + K^A_{iz,f}\right)\right] - S_f(h_f) - \frac{\Gamma_w}{w} \\ \frac{\partial \theta_m(h_m)}{\partial t} &= \frac{\partial}{\partial x_i}\left[K_m(h_m)\left(K^A_{ij,m}\frac{\partial h_m}{\partial x_j} + K^A_{iz,m}\right)\right] - S_m(h_m) + \frac{\Gamma_w}{1-w}\end{aligned} \tag{1}$$

where subscripts *f* and *m* refer to the fracture and matrix domains, w is the ratio of the volumes of the macropore or fracture domain and the total soil system [-], θ is the volumetric water content [L^3L^{-3}], h is the pressure head [L], S is a sink term [T^{-1}], x_i (i=1,2) are the spatial coordinates [L], t is time [T], Γ_w is the transfer rate for water from the inter- to the intra-aggregate pores, K_{ij}^A are components of a dimensionless anisotropy tensor $\mathbf{K}^A$, and K is the unsaturated hydraulic conductivity function [LT^{-1}] given by

$$K(h, x, y, z) = K_s(x, y, z)\, K_r(h, x, y, z) \tag{2}$$

where K_r is the relative hydraulic conductivity and K_s the saturated hydraulic conductivity [LT^{-1}]. The anisotropy tensor K_{ij}^A in (1), which can be different for the two domains, is used to account for an anisotropic medium. The diagonal entries of K_{ij}^A equal one and the off-diagonal entries zero for an isotropic medium. If (1) is applied to planar flow in a vertical cross-section, x_1=x is the horizontal coordinate and x_2=z is the vertical coordinate, the latter taken to be positive upward. Einstein's summation convention is used in (1) and throughout this report. Hence, when an index appears twice in an algebraic term, this particular term must be summed over all possible values of the index.

Solutions of the Richards equation (1) require knowledge of the unsaturated soil hydraulic functions made up of the soil water retention curve, $\theta(h)$, which describes the relationship between the water content θ and the pressure head h, and the unsaturated hydraulic conductivity function, $K(h)$, which defines the hydraulic conductivity K as a function of h or θ. The dual-permeability approach, as developed by *Gerke and van Genuchten* [1993a], 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 a hydraulic

conductivity function of the fracture-matrix interface. Note that the water contents θ_f and θ_m in (1) have different meanings than in the dual-porosity model where they represented water contents of the total pore space (i.e., $\theta = \theta_{mo} + \theta_{im}$), while here they refer to water contents of the two separate (fracture or matrix) pore domains such that

$$\theta = \theta_F + \theta_M = w\theta_f + (1-w)\theta_m \tag{3}$$

Hence, lower case subscripts in the dual-permeability model refer to the local (pore-region) scale, while upper case subscripts refer to the global (total soil medium) scale.

2.2. *Water Mass Transfer*

The rate of exchange of water between the fracture and matrix regions, Γ_w, is usually assumed to be proportional to the difference in pressure heads between the two pore regions [*Gerke and van Genuchten*, 1993a]:

$$\Gamma_w = \alpha_w (h_f - h_m) \tag{4}$$

in which α_w is a first-order mass transfer coefficient [$L^{-1}T^{-1}$]. Since pressure heads are now needed for both regions, this approach requires retention curves for both pore regions. For porous media with well-defined geometries, the first-order mass transfer coefficient, α_w, can be defined as follows [*Gerke and van Genuchten*, 1993b]:

$$\alpha_w = \frac{\beta}{d^2} K_a \gamma_w \tag{5}$$

where d is an effective 'diffusion' pathlength (i.e. half the aggregate width or half the fracture spacing) [L], β is a shape factor that depends on the geometry [-], and γ_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 value of β varies with the geometry assumed for the aggregates [*van Genuchten and Dalton*, 1986]; it is 3 for rectangular slabs. *Gerke and van Genuchten* [1996] suggested a method for deriving values of the shape factor β in (5) for non-idealized geometries or mixtures of shapes in order to obtain a more general 'macroscopic' approach. *Gerke and van Genuchten* [1996] evaluated the effective hydraulic conductivity K_a [LT^{-1}] of the fracture-matrix interface using a simple arithmetic average involving both h_f and h_m as follows

$$K_a(h) = 0.5\left[K_a(h_f) + K_a(h_m)\right] \tag{6}$$

The use of (6) implies that the medium contains geometrically well-defined rectangular or other types of macropores or fractures (e.g. *Edwards et al.* [1979], *van Genuchten and Dalton* [1986], and *Gerke and van Genuchten* [1996]). 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 (6) may not be identifiable. Hence, rather than using (6) directly, one could also lump β, d, and γ_w into one effective hydraulic conductivity K_a^* of the fracture-matrix interface to give

$$\alpha_w = K_a^*(h) \tag{7}$$

in which case Ka* can be used as a calibration parameter.

2.3. *Soil Hydraulic Properties*

The unsaturated soil hydraulic properties, $\theta(h)$ and $K(h)$, in (1) are in general highly nonlinear functions of the pressure head. The DualPerm module of HYDRUS implements the soil-hydraulic functions of *van Genuchten* [1980] who used the statistical pore-size distribution model of *Mualem* [1976] to obtain a predictive equation for the unsaturated hydraulic conductivity function in terms of soil water retention parameters. The expressions of *van Genuchten* [1980] are given by

$$\theta(h) = \begin{cases} \theta_r + \dfrac{\theta_s - \theta_r}{[1+|\alpha h|^n]^m} & h < 0 \\ \theta_s & h \geq 0 \end{cases} \tag{8}$$

$$K(h) = K_s S_e^l [1 - (1 - S_e^{1/m})^m]^2 \tag{9}$$

where

$$m = 1 - 1/n \ , \quad n > 1 \tag{10}$$

The above equations contain six independent parameters: θ_r, θ_s, α, n, K_s, and l. The pore-connectivity parameter l in the hydraulic conductivity function was estimated [*Mualem*, 1976] to be about 0.5 as an average for many soils. These soil hydraulic functions are used for both the matrix and fracture domains.

3. Dual-Permeability Solute Transport

3.1. *Governing Solute Transport Equation*

Analogous to Eq. (1), the dual-permeability formulation for solute transport is based on advection-dispersion type equations for transport in both the fracture and matrix regions as follows [*Gerke and van Genuchten*, 1993a] (Fig. 1):

$$\begin{aligned}\frac{\partial \theta_f c_f}{\partial t} + \rho \frac{\partial s_f}{\partial t} &= \frac{\partial}{\partial x_i}\left(\theta_f D_{ij}^f \frac{\partial c_f}{\partial x_j} \right) - \frac{\partial q_{f,i} c_f}{\partial x_i} - \phi_f - \frac{\Gamma_s}{w} \\ \frac{\partial \theta_m c_m}{\partial t} + \rho \frac{\partial s_m}{\partial t} &= \frac{\partial}{\partial x_i}\left(\theta_m D_{ij}^m \frac{\partial c_m}{\partial x_j} \right) - \frac{\partial q_{m,i} c_m}{\partial x_i} - \phi_m + \frac{\Gamma_s}{1-w}\end{aligned} \tag{11}$$

where subscripts *f* and *m* again refer to the fracture and matrix domains, *c* and *s* are solute concentrations in the liquid [ML^{-3}] and solid [MM^{-1}] phases, respectively; *q* is the volumetric flux density [LT^{-1}], ρ is the soil bulk density [$M\ L^{-3}$], D_{ij} is the dispersion coefficient tensor [L^2T^{-1}] for the liquid phase, Γ_s is the mass transfer term for solute exchange between the fracture and matrix domains [$ML^{-3}T^{-1}$], and ϕ represents the sink/source term, accounting for first-order degradation and zero-order production processes, as well as root solute uptake. The first equation of (11) describes solute transport in the fracture domain, the second equation transport in the matrix domain. Equation (11) assume complete advective-dispersive transport descriptions for both the fractures and the matrix.

Similarly as in the standard solute transport model of HYDRUS (2D/3D), the solute transport model in the dual-permeability module can be linked with the chemical nonequilibrium two-site sorption model or the physical nonequilibrium dual-porosity (mobile-immobile water) model. For governing equations of these two nonequilibrium models, see the technical manual of HYDRUS (2D/3D) [*Šimůnek et al.*, 2011].

3.2. *Solute Mass Transfer*

The advective-dispersive mass transfer between the fracture and matrix domains is traditionally described using the following form:

$$\Gamma_s = \alpha_s (1-w)\theta_m (c_f - c_m) + \Gamma_w c^* \tag{12}$$

where α_s is the first-order solute mass transfer coefficient [T^{-1}] accounting for physical rate process. c^* in (12) is equal to c_f for $\Gamma_w>0$ and c_m for $\Gamma_w<0$. *van Genuchten and Dalton* [1986] and *Gerke and van Genuchten* [1996], among others, discussed possible expressions for the first-order solute mass transfer coefficient, α_s [T^{-1}], which can be defined as:

$$\alpha_s = \frac{\beta}{d^2} D_a \tag{28}$$

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

4. Preprocessing and Input Data

4.1. *Soil Hydraulic Model*

The Dual-Permeability module is activated when the "**Dual-Permeability**" check box is selected in the **Soil Hydraulic Model** window (Fig. 2). Once this check box is selected, the edit box "**Fraction of Boundary Flux into Fracture**" appears. The value of this parameter can be specified by a user and should vary between 0 and 1. When 0 is specified, all water at boundaries with a specified boundary flux will enter into the matrix. When 1 is specified, all water at boundaries with a specified boundary flux will enter into the fracture domain.

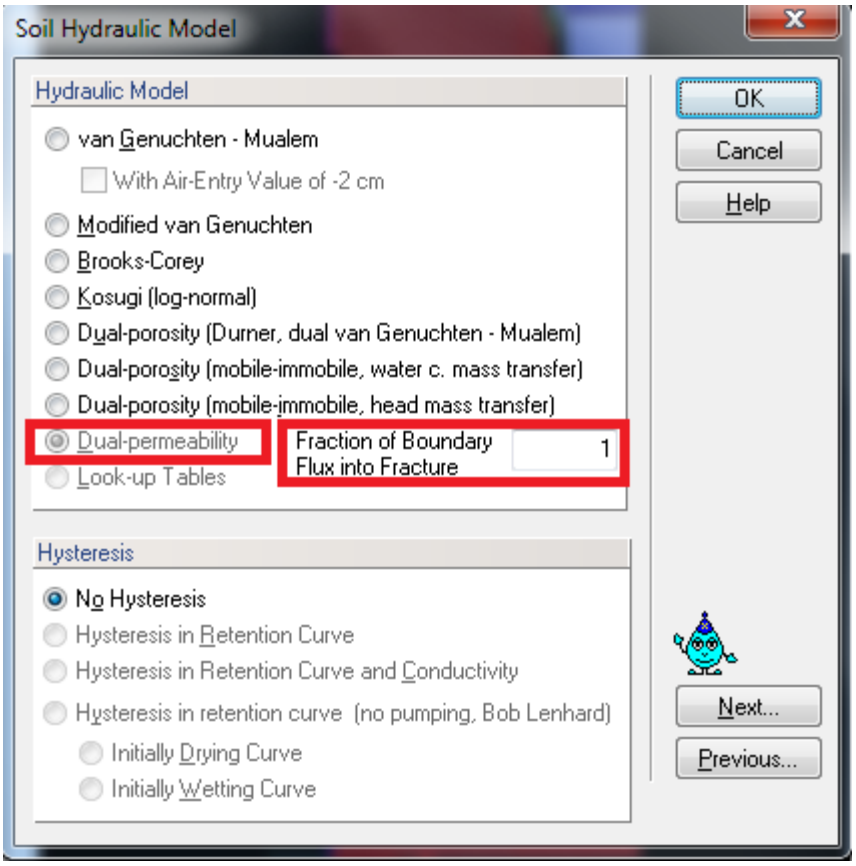

Figure 2. The Soil Hydraulic Model dialog window.

4.2. *Water Flow Parameters*

The soil hydraulic parameters for the dual-permeability module are specified in the **Water Flow Parameters** window (Fig. 3). Six soil hydraulic parameters (θ_r, θ_s, α, n, K_s, and l) are needed for both the matrix and fracture domains to describe the retention curve and hydraulic conductivity function. Additional 5 parameters are needed to characterize the matrix-fracture interface (w, β, γ_w, d, and K_{as}). Detailed description of all soil hydraulic parameters is given in Table 1.

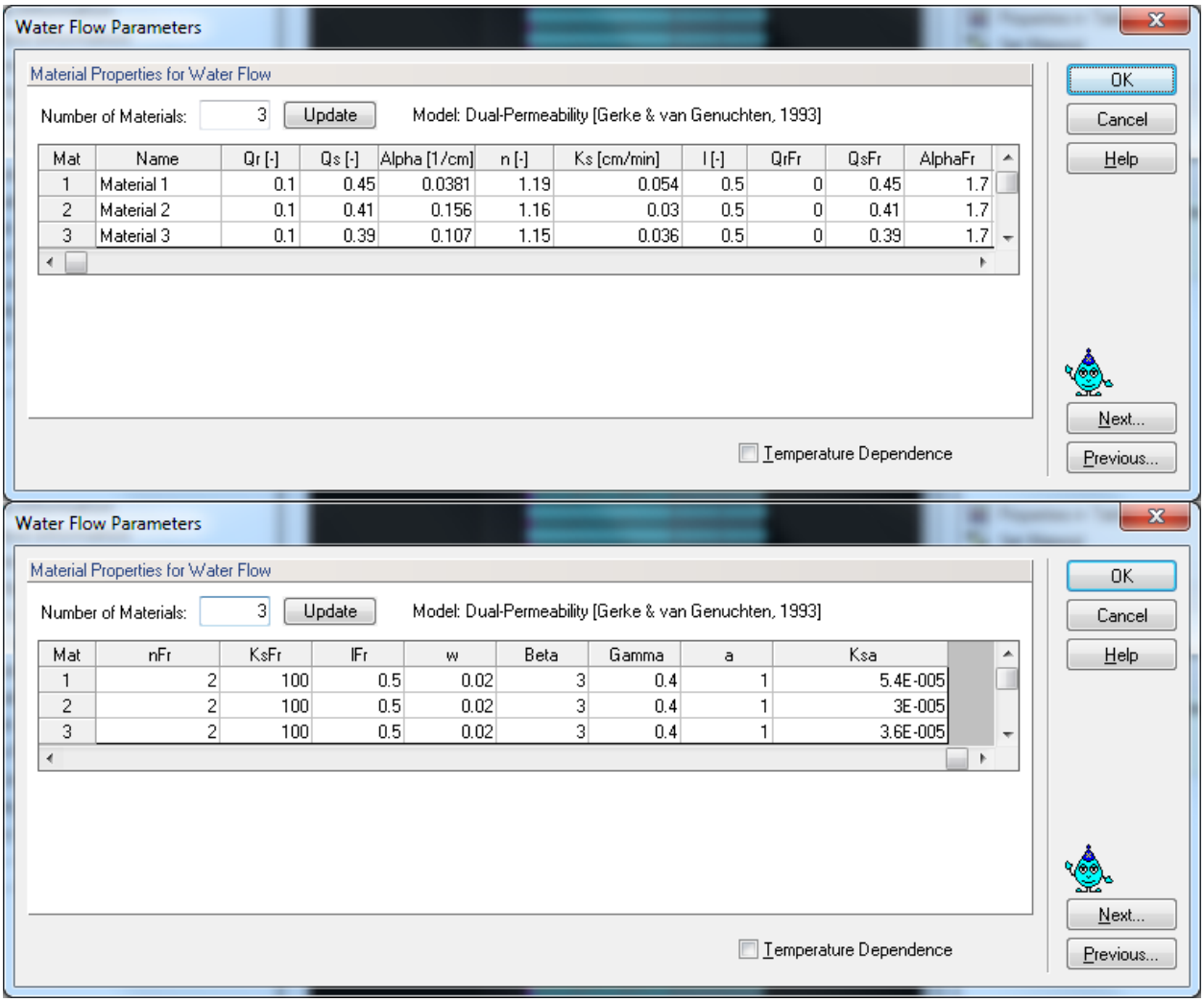

Figure 3. The Water Flow Parameters dialog window (for three materials).

Table 1. Water flow parameters for the dual-permeability module.

Parameter	Notation	Description
Qr	θ_r	Residual soil water content of the matrix [L^3/L^3] (see eq. (8)).
Qs	θ_s	Saturated soil water content of the matrix [L^3/L^3].
Alpha	α	Parameter α in the soil water retention function of the matrix [L^{-1}].
n	n	Parameter n in the soil water retention function of the matrix [-].
Ks	K_s	Saturated hydraulic conductivity of the matrix [LT^{-1}].
l	l	Tortuosity parameter in the conductivity function of the matrix [-].
QrFr	θ_r	Residual soil water content of the fracture domain [L^3/L^3].
QsFr	θ_s	Saturated soil water content of the fracture domain [L^3/L^3].
AlphaFr	α	Parameter α in the soil water retention function of the fracture domain

		[L^{-1}].
nFr	n	Parameter n in the soil water retention function of the fracture domain [-].
KsFr	K_s	Saturated hydraulic conductivity of the fracture domain [LT^{-1}].
lFr	l	Tortuosity parameter in the conductivity function of the fracture domain [-].
w	w	Ratio of the volumes of the macropore or fracture domain and the total soil system [-] (see eq. (5)). Must be the same for all soil layers.
Beta	β	Shape factor that depends on the geometry [-] (see eq. (5)); it is 3 for rectangular slabs.
Gamma	γ_w	Scaling factor (=0.4) [-] (see eq. (5)).
a	d	Effective 'diffusion' pathlength (i.e. half the aggregate width or half the fracture spacing) [L] (see eq. (5)).
Ksa	K_{as}	Saturated hydraulic conductivity K_{as} [LT^{-1}] of the fracture-matrix interface (see eqs. (5) and (6)).

4.3. *Solute Transport Parameters*

The solute transport parameters for the dual-permeability module are specified in the **Solute Transport Parameters** window (Fig. 4). Detailed description of these parameters is given in Tables 2 and 3.

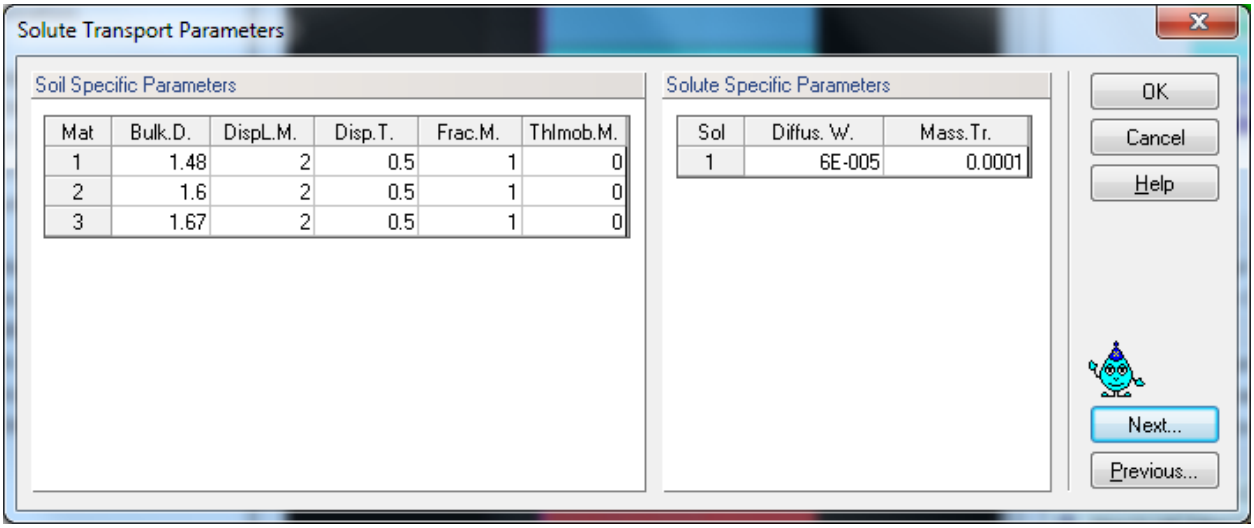

Figure 4. The Solute Transport Parameters dialog window.

a) Soil Specific Parameters

These parameters are common for all three components, but different for different soil layers.

Table 2. Soil specific solute transport parameters.

Parameter	Notation	Description
Bulk. D.	ρ	Bulk density [M/L^3]
DispL.M.	λ_L	Longitudinal dispersivity in the matrix domain [L]
Disp.T.	λ_T	Transverse dispersivity [L]
Fract.M	f	Dimensionless fraction of adsorption sites classified as type-1 sites, i.e., sites with instantaneous sorption when the **chemical nonequilibrium** option is considered [-] in the matrix domain. Set this parameter equal to 1 when equilibrium transport is considered. *Frac* becomes the dimensionless fraction of adsorption sites in contact with mobile water when the **physical nonequilibrium** option is considered [-]. In that case *Frac* should be set equal to 1 when all sorption sites are in contact with mobile water.
ThImob.M.	θ_{im}	Immobile water content in the matrix domain. Set equal to 0 when the **physical nonequilibrium** option is not considered.

b) Solute Specific Parameters

These parameters are common for different soil layers, but may be different for different components.

Table 3. Solute specific solute transport parameters.

Parameter	Notation	Description
Diffus. W.	D_w	Molecular diffusion in the liquid phase [LT^{-2}]
Mass.Tr.	D_a	Effective diffusion coefficient [L^{2}T^{-1}], which represents the diffusion properties of the fracture-matrix interface as well as other parameters.

4.4. *Solute Reaction Parameters*

The solute transport parameters for the dual-permeability module are specified in the **Solute Reaction Parameters** window (Fig. 5). Detailed description of these parameters is given in Tables 4.

Table 4. Solute Reaction parameters.

Parameter	Notation	Description
KdM	K_d	Adsorption isotherm (distribution) coefficient for the matrix [M^{-1}L^3].
Nu	η	Adsorption isotherm (Langmuir) coefficient [L^3/M] (used for both matrix and fracture domains).
Beta	β	Adsorption isotherm (Freundlich) exponent [-] (used for both matrix and fracture domains).
AlphaM	ω	First-order rate coefficient for nonequilibrium adsorption in the matrix

		[T^{-1}].
SinkL1	μ_w	First-order degradation rate constant for dissolved phase [T^{-1}] (used for both matrix and fracture domains).
SinkS1	μ_s	First-order degradation rate constant for solid phase [T^{-1}] (used for both matrix and fracture domains).
Disp.F.	λ_L	Longitudinal dispersivity in the fracture domain [L]
SinkL1'	μ_w'	First-order degradation rate constant (representing the chain reaction) for dissolved phase [T^{-1}] (used for both matrix and fracture domains).
SinkS1'	μ_s'	First-order degradation rate constant (representing the chain reaction) for solid phase [T^{-1}] (used for both matrix and fracture domains).
Frac.F.	f	Dimensionless fraction of adsorption sites classified as type-1 sites, i.e., sites with instantaneous sorption when the **chemical nonequilibrium** option is considered [-] in the fracture domain. Set this parameter equal to 1 when equilibrium transport is considered. *Frac* becomes the dimensionless fraction of adsorption sites in contact with mobile water when the **physical nonequilibrium** option is considered [-]. In that case *Frac* should be set equal to 1 when all sorption sites are in contact with mobile water.
SinkL0	γ_w	Zero-order (production) rate constant for dissolved phase [$ML^{-3}T^{-1}$].
SinkS0	γ_s	Zero-order (production) rate constant for solid phase [T^{-1}].
KdF	K_d	Adsorption isotherm (distribution) coefficient for the fracture domain [$M^{-1}L^3$].
AlphaF	ω	First-order rate coefficient for nonequilibrium adsorption in the fracture domain [T^{-1}].

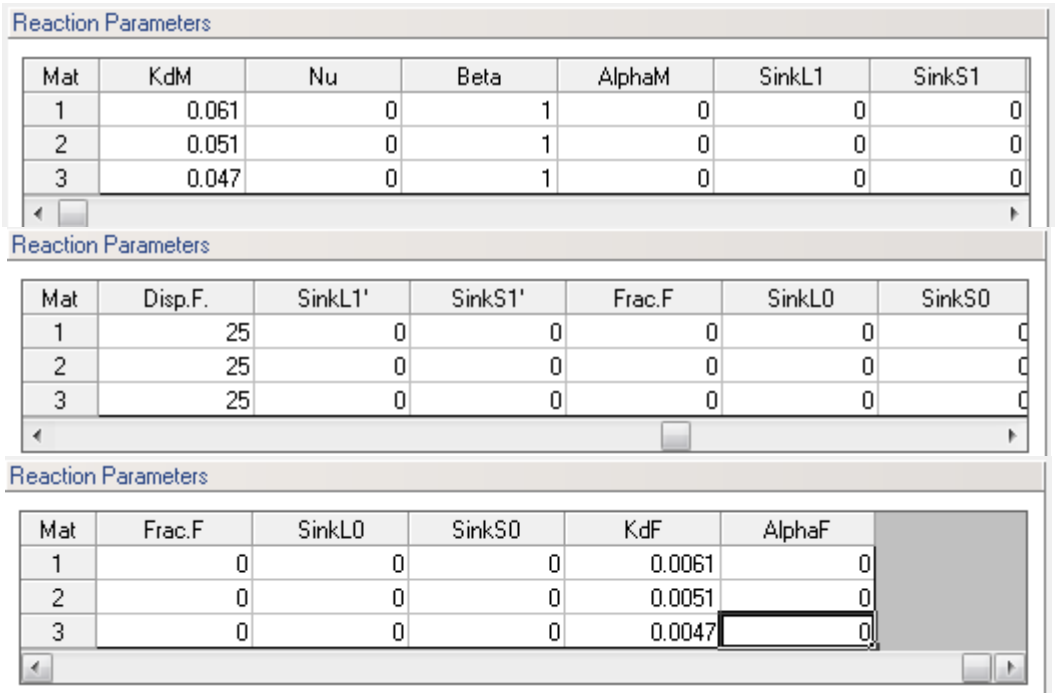

Figure 5. Parts of the "Reaction Parameters for Solute -1" dialog window (for three materials).

4.5. *Initial Conditions*

Initial conditions for water flow can be specified either in terms of pressure heads or water contents. When the pressure head is used to specify the initial conditions, the same pressure head is used in both matrix and fracture domains (i.e., it is assumed that the two domains are in equilibrium). When the water content is used to specify the initial conditions, the specified water content is assigned to the matrix domain, and the corresponding pressure head (calculated from the retention curve of the matrix domain) is assigned to both the matrix and fracture domains. The same initial concentrations are assumed for both the matrix and transport domains.

4.6. *Anisotropy*

In the standard HYDRUS code, the angle of anisotropy, and the 1st and 2nd component of the anisotropy tensor K_{ij}^{A} are specified in GUI. In the DualPerm module, this input is reinterpreted for the two (matrix and fracture) domains differently. The angle of anisotropy (**Anisotropy - Angle**; Fig. 6) must be the same in both transport domains. The input "**Anisotropy - 1st Component**" (Fig. 6) is interpreted as a ratio of the horizontal and vertical components (K_x^A/K_z^A) of the anisotropy tensor of the matrix domain, while the input "**Anisotropy - 2st Component**" (Fig. 6) is interpreted as a ratio of the horizontal and vertical components (K_x^A/K_z^A) of the anisotropy tensor of the fracture domain.

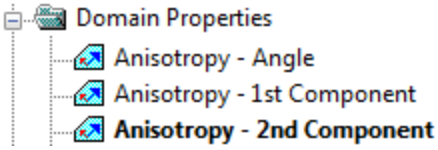

Figure 6. The "Domain Properties" part of the Data Tab of the Navigator Bar.

5. Post-processing

5.1. *Results – Graphical Display*

Multiple outputs from the DualPerm module are duplicated for the matrix and fracture domains (Table 5). Each of these outputs can be displayed as done in the standard HYDRUS version by clicking on corresponding commands in the "Results - Graphical Display" (Fig. 7) and "Results - Other Information" parts of the Navigator bar. Matrix or fracture information is displayed depending on the "**Dual-Permeability Options**" switch (**Display Matrix** or **Display Fractures**) that can be selected either in the "Results" part of the View Tab of the Navigator Bar (Fig. 8) or on the Edit (Tools) Bar (Fig. 9). In addition to the standard output, water and solute mass transfer between the matrix and fracture domains can be also displayed (Fig. 7).

Table 5. Duplicated outputs from the DualPerm module for the matrix and fracture domains.

File	Description
h.out and hF.out	Nodal values of pressure heads in the matrix and fracture domains.
th.out and thF.out	Nodal values of water contents in the matrix and fracture domains.
v.out and vF.out	Nodal values of fluxes in the matrix and fracture domains.
Conc1.out and ConcF1.out	Nodal values of concentrations in the matrix and fracture domains.
ObsNod.out and ObsNodF.out	Observation node values of pressure heads, water contents, and concentrations in the matrix and fracture domains.
Solute1.out and SoluteF1.out	Boundary and reaction solute fluxes for the matrix and fracture domains.

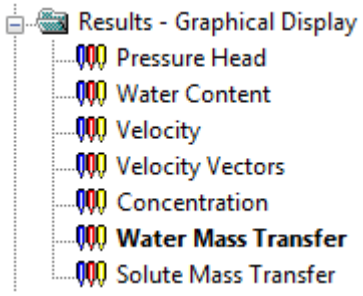

Figure 7. The "Results - Graphical Display" part of the Data Tab of the Navigator Bar.

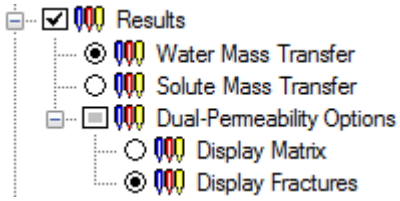

Figure 8. The "Results" part of the View Tab of the Navigator Bar.

Figure 9. The "Dual-Permeability Options" switch at the Edit (Tools) Bar.

5.2. *The v_meanF.out Output File*

An additional output file v_meanF.out is created, which is not recognized by GUI and which provides information about various actual and cumulative boundary fluxes and average pressure heads for the fracture domain (Table 6).

Table 6. The v_meanF.out output file.

Variable	**Description**
t	Time
vFrac	Water mass transfer between the fracture and matrix domain [L/T]
CumFrac	Cumulative water mass transfer between the fracture and matrix domain [L]
vFracS	Solute mass transfer between the fracture and matrix domain [M/L^2/T]
vCumFracs	Cumulative solute mass transfer between the fracture and matrix domain [M/L^2]
vMeanF(iKod)	Water flux across the boundary with Kode=iKod [L^2/T] (iKod=1: constant head or flux boundary; =2: seepage face; =3: variable head or flux; =4: atmospheric; =5: drains; =6: free or deep drainage.
CumQF(iKod)	Cumulative water flux across the boundary with Kode=iKod [L^2]
hMeaF(iKod)	Average pressure head at the boundary with Kode=iKod [L]

6. Example Problems

The DualPerm module supplements the standard HYDRUS program, which includes variably-saturated water flow and solute transport model, and thus the water flow and solute transport parts of the model have been widely tested earlier. Therefore, verification and test examples presented in this section concentrate on the demonstration of the new features of the model.

The new module and most of its new features have been extensively tested on test problems of increasing complexity (Table 7). The first set of examples described in Sections 6.1 and 6.2 (Test1a through Test1f; see Table 7) considered surface flux either into the fracture (Section 6.1) or matrix (Section 6.2) domain and different sizes of the aggregates (parameter *d*). The second test of examples (Test2a through Test2f) considered surface ponding. The third test of examples (Test3 through Test3b) simulated tension disc infiltration experiment, considering either isotropic or anisotropic fracture domain. The final two examples (DPerm_2SM and DPerm_MIM) considered, in addition to the dual-permeability medium, also the nonequilibrium problem in one (immobile water in the matrix) or both (two-site sorption) domains.

Table 7. List of various test examples used to verify various new options of the DulPerm module.

Name	**Solute**	**Description**
Test1a	No	Flux upper BC. Flux into fracture, *d*=1.0 cm.
Test1a1	No	Flux upper BC. Flux into matrix, *d*=1.0 cm.
Test1a2	No	Flux upper BC. Flux into matrix, *d*=1.0 cm. Higher flux.
Test1a3	Yes	Flux upper BC. Flux into matrix, *d*=1.0 cm. Solute.
Test1a4	No	Atmospheric upper BC. Root uptake, *d*=1.0 cm.
Test1b	No	Flux upper BC. Flux into fracture, *d*=0.1 cm.
Test1c	No	Flux upper BC. Flux into fracture, *d*=0.0316 cm.
Test1d	Yes	Flux upper BC. Flux into fracture, *d*=1.0 cm. Solute.
Test1d1	Yes	Flux upper BC. Flux into fracture, *d*=1.0 cm. Solute inflow.
Test1e	Yes	Flux upper BC. Flux into fracture, *d*=0.1 cm. Solute.
Test1f	Yes	Flux upper BC. Flux into fracture, *d*=0.0316 cm. Solute.
Test2a	No	Surface ponding, *d*=1.0 cm.
Test2b	No	Surface ponding, *d*=0.2 cm.
Test2c	No	Surface ponding, *d*=3.0 cm.
Test2d	Yes	Surface ponding, *d*=1.0 cm, solute.
Test2e	Yes	Surface ponding, *d*=0.2 cm, solute.
Test2f	Yes	Surface ponding, *d*=3.0 cm, solute.
Test3	Yes	Ring infiltration into the isotropic dual-permeability system.
Test3a	Yes	Ring infiltration into dual-permeability system; different anisotropy in fracture (10:1) and matrix (1:1) domains.
Test3b	Yes	Ring infiltration into dual-permeability system; different anisotropy in Fracture (1:10) and Matrix (1:1) domains.
DPerm_2SM	Yes	Dual-permeability model, two-site sorption model.
DPerm_MIM	Yes	Dual-permeability model, dual-porosity (MIM) in matrix.

6.1. *Example 1 (Test1d): Surface Flux Into Fracture*

This example demonstrates the application of the dual-permeability model of *Gerke and van Genuchten* [1993a] to infiltration into a macroporous soil profile 40 cm deep. The following soil hydraulic parameters for the matrix (θ_r=0.105, θ_s=0.50, α_1=0.005 cm^{-1}, n=1.5, l=0.5, K_s=1.05 cm d^{-1}), the fracture (θ_r=0.0, θ_s=0.50, α_1=0.1 cm^{-1}, n=2.0, l=0.5, K_s=2000.0 cm d^{-1}), and the matrix-fracture interface (w=0.05, β=3, γ=0.4, a=1.0, and K_{as}=0.01 cm d^{-1}, see Eq. (5) above) were used. Water mass transfer was described using Eq. (4). Only convective solute mass transfer between the two pore regions, with a dispersivity of 2 cm, was considered. The initial pressure head for both regions was equal to –1000 cm, while water was applied only to the soil fracture.

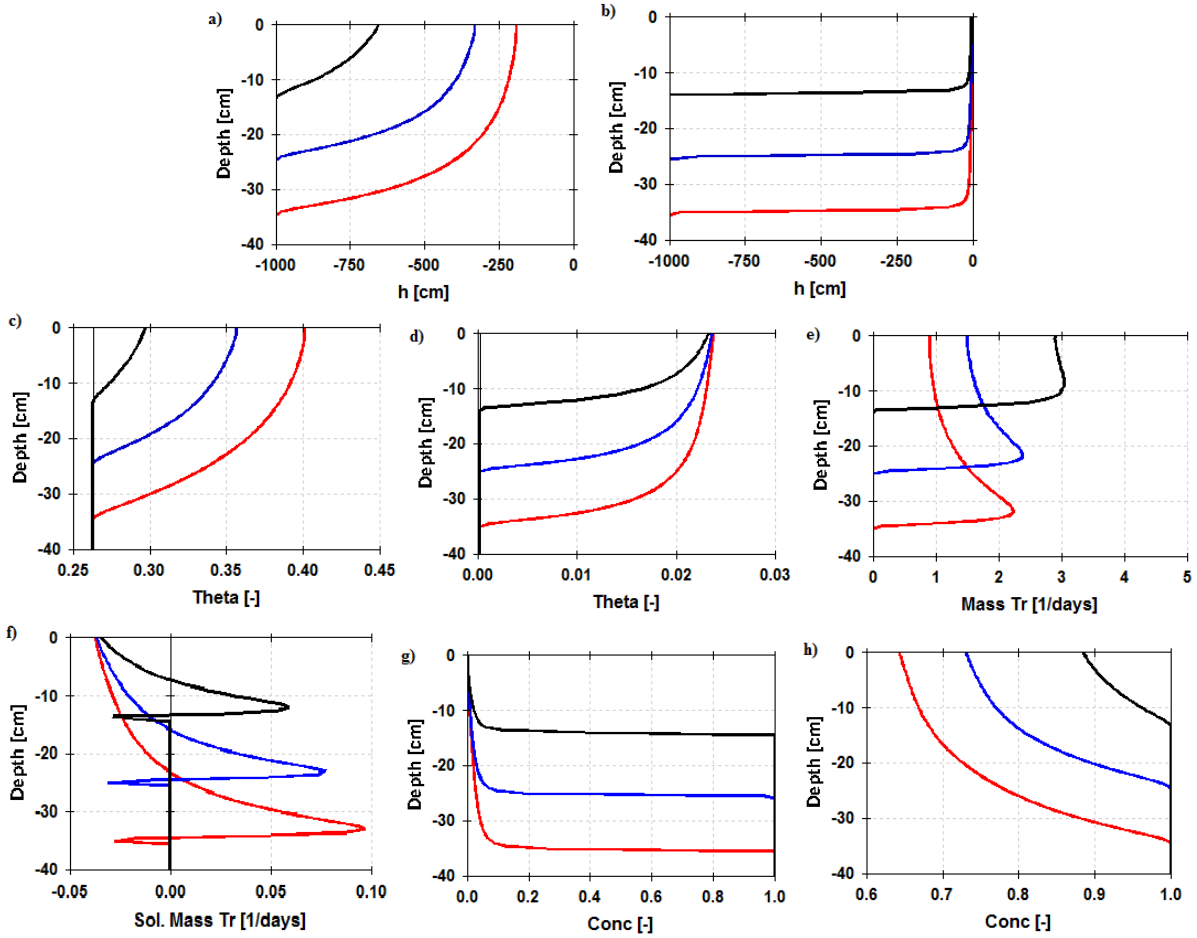

Figure 10. Pressure heads in the matrix (a) and fracture (b) domains, water contents in the matrix (c) and fracture (d) domains, water mass exchange rates (e), solute mass exchange rates (f), and concentrations in the matrix (h) and fracture (g) domains calculated with the dual-permeability model of *Gerke and van Genuchten* [1993a,b].

6.2. *Example 2 (Test1a3): Surface Flux Into Matrix*

This example was taken from *Šimůnek et al.* [2003]. Figure 11 shows an application of the dual-permeability model of *Gerke and van Genuchten* [1993a] to infiltration into a macroporous soil profile 40 cm deep. The same system and the same parameters were used as above (example 1) except that 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 cm d^{-1}) greatly exceeded the saturated hydraulic conductivity of the matrix (K_s = 1.05 cm d^{-1}) (Fig. 11a). Water started to flow into the fracture domain (Fig. 10a) where it moved vertically downwards (Fig. 11c) and infiltrated into the matrix domain (Fig. 10d). The two distinct moisture fronts in Figure 11b (and concentration fronts in Figure 11e) are due to lateral transfer from the fracture domain (the leading edge), and flow in the matrix domain (the second front).

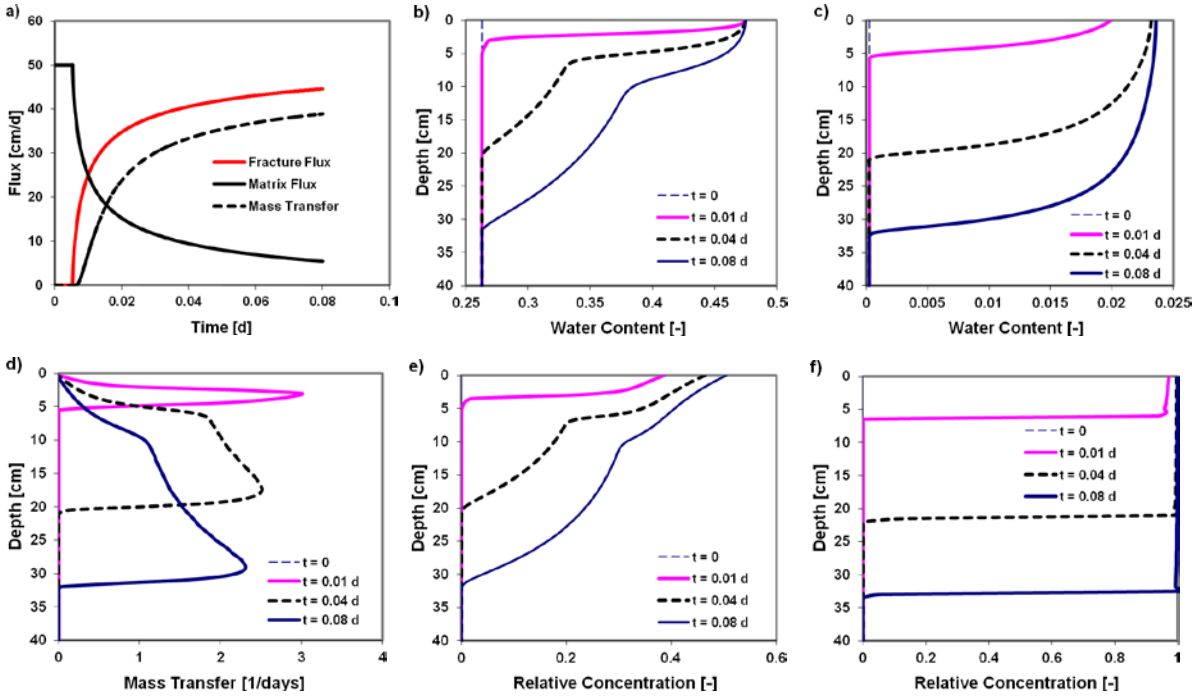

Figure 11. Infiltration and mass exchange fluxes (a), water contents in the matrix (b) and fracture (c) domains, water mass exchange rates (d) and concentrations in the matrix (e) and fracture (f) domains calculated with the dual-permeability model of *Gerke and van Genuchten* [1993a,b].

6.3. *Examples 3 (Test3) - Tension Disc Infiltration Experiment*

The tension disc infiltration experiment (with a disc radius of 10 cm) is simulated in this test example. The axisymmetrical transport domain is 50 cm wide and 150 cm deep. The soil profile is assumed to consist of three soil layers (with each upper layers 20 cm thick). The soil hydraulic and solute transport and reaction parameters are shown above in Figures 3, 4, and 5. The solute free, equilibrium initial profile with groundwater table at the bottom of the soil profile is considered. The tension applied at the disc is -0.4 cm. The soil matrix is considered to be isotropic, while the fracture domain is assumed to be either isotropic, or to have the ratio K_x^A/K_z^A equal to 10 or 0.1. Pressure head profiles for these three conditions with different anisotropies of the fracture domain are shown in Figure 12. Note that while we shoe in Figure 12a the pressure head profile in the matrix only for the first scenario (i.e., both domains are isotropic), the matrix pressure head profiles for the other scenarios are not very different.

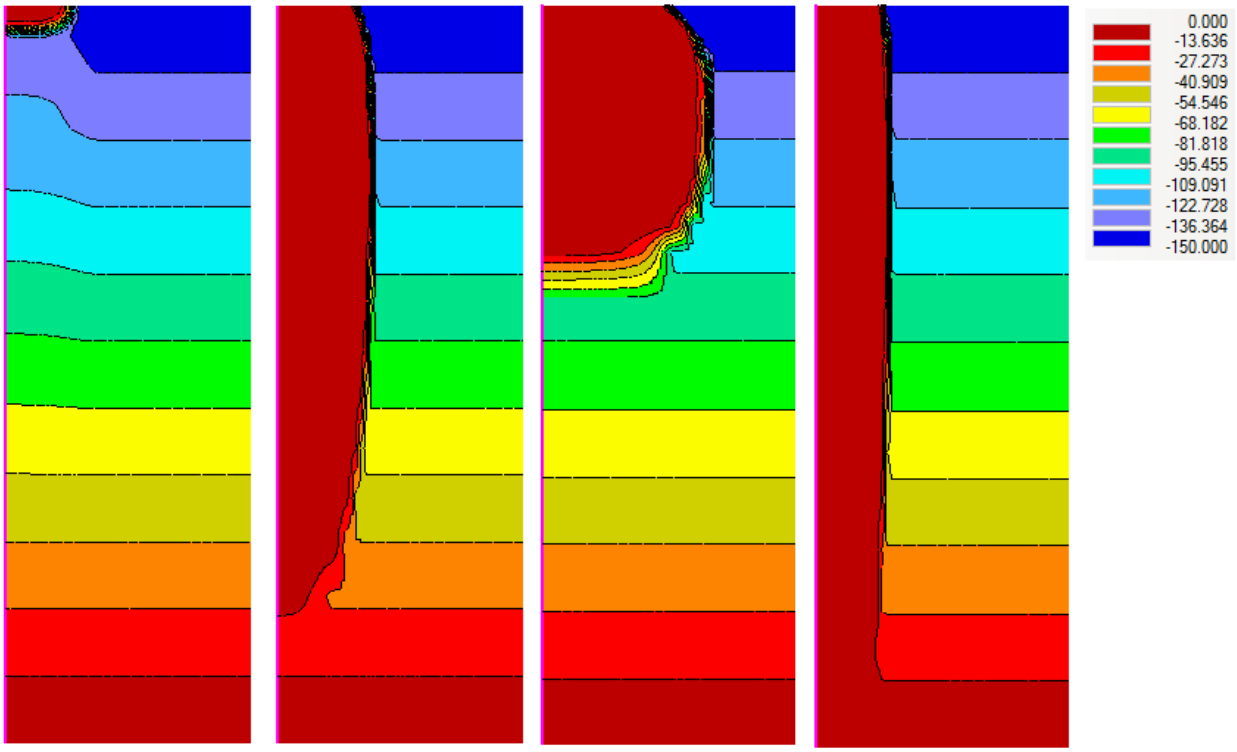

Figure 12. Pressure head profiles for the matrix, isotropic fracture, and fracture with K_x^A/K_z^A=10, and fracture with K_x^A/K_z^A=0.1 after 19 minutes.

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