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Parameter estimation for a double continuum transport model for fractured porous media

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Abstract To predict plume development in fractured matrix systems without detailed knowledge of the fracture network geometries, a double continuum approach is chosen. The complex transport behaviour can be adequately represented by two overlapping and interacting continua. An existing double continuum approach has been further developed for steady-state flow conditions, with the focus on the mass exchange terms between the fractures and the matrix system. This approach is implemented in the "Double Porosity MT3D" program and has been applied to a transport problem in a fractured porous system. The parameter determination for the fracture continuum is the most important step for calibrating the double continuum model and predicting the plume development adequately. Of particular interest was the determination of hydraulic parameters by fracture network characteristics. The transversal dispersion coefficient and hydraulic conductivity are directly dependent on the angles between the fracture directions and hydraulic gradient. The larger the angle, the higher is the transversal dispersion coefficient and the lower will be the resulting effective hydraulic conductivity.

Keywords double continuum model; fracture networks; transport simulation

INTRODUCTION

The determination of plume developments in fractured porous media is very complicated due to their extremely complex structure. Large fractures provide preferential pathways for regional fluid movement leading to a fast contaminant transport, whereas the small fractures as well as the rock matrix are relevant in terms of storage and retardation, as their permeability values are some orders of magnitude smaller. The interactions between these parts of the system are characterized by specific exchange processes. The main exchange processes are given by matrix diffusion as a result of concentration differences between the fractures and matrix, local advection due to pressure gradients between the fractures and matrix, and regional advection due to a regional pressure gradient.

To describe flow and transport processes in fractured porous media, several model approaches are available depending on the scale of application and geological information (Fig. 1). The simplest approach, single continuum representation, can be used for macroscale studies, if a rough approximation is sufficient without representing the complex structure of the system.

A much better representation of the complex system can be achieved by applying discrete approaches. Due to the fact, that for useful modelling results the exact geometry of all individual fractures has to be determined, the computational effort is

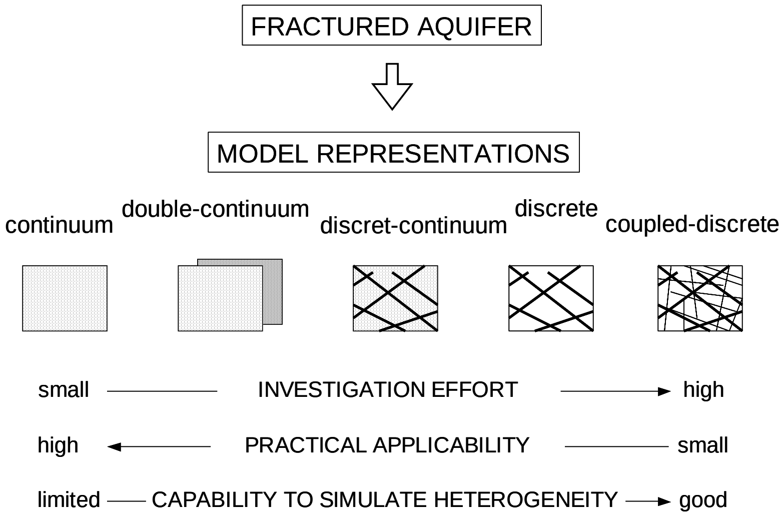

Fig. 1 Different model representations for fractured aquifers (after Teutsch & Sauter, 1991).

very high. For this reason the discrete approaches are limited to local scale studies of well known investigation areas.

A combination of discrete and continuum approaches can be used for investigations where some known large fractures dominate the system. If a fractured porous medium should be described without considering the exact fracture network geometries, a double continuum approach can be chosen. The fractured porous medium is described by two overlapping and interacting continua. The first continuum represents the large fracture system, whereas the second continuum represents the small fracture system or the matrix, respectively. These two continua possess different flow, transport and storage parameters and are connected by respective exchange terms. Detailed knowledge of the fracture network geometries is not required, but the complex transport behaviour can be adequately represented. In general two different types of double continuum approaches are known. Within the dual porosity approach only one continuum contributes to the regional flow, whereas the second continuum is just a fluid and solute storage. A dual permeability approach consists of two continua which both contribute to the regional flow.

DOUBLE CONTINUUM APPROACH

For the presented investigations the 3-D double continuum program package DP-MODFLOW was chosen; it was first introduced by Teutsch & Sauter (1991). This program package is based on the well known 3-D-finite-difference model MODFLOW (McDonald & Harbaugh, 1984) and MT3D, as they were suitable for extending because of their modular structure. The flow and transport simulations can be calculated for each continuum by solving the universally valid flow and transport differential equations. The flow and transport exchange formulations of the two continua are very important for the success of the simulation. Subsequently, only the transport exchange terms are described, as the flow exchange is assumed to be already solved (Lang, 1995; Mohrlok, 1996).

As mentioned above, matrix diffusion, local advection and regional advection, being the three main exchange processes, have to be taken into account. Lang (1995) defined the local advection term as:

$$q_{ex,la} = \alpha_0 (h^a - h^b) C^{a,b} \quad (1)$$

where α_0 is the hydraulic exchange coefficient, (h^a – h^b) is the piezometric head difference between the continua and $C^{a,b}$ is the concentration of the continuum *a* or *b*.

For steady-state flow conditions, the exchange between the continua is dominated by the regional advection, which depends on the angles between the fracture directions and hydraulic gradient. This process follows the regional pressure gradient. Thereby, the exchange volume is dependent on the velocity within the matrix and the fracture surface which is perpendicular to the flow direction. Birkhölzer (1994) defined the regional advection term as:

$$q_{ex,ra} = (1 - n^a) \left| q_i^b \right| \Omega_W \quad (2)$$

where n^a is the effective porosity of the fracture continuum, q^b the effective velocity of the matrix continuum, and Ω_W the specific fracture surface as a function of the relevant fracture surface and the matrix volume. This regional advection term was implemented within DP-MT3D model for the present investigations.

Since DP-MT3D is based on the dual-permeability approach, the matrix diffusion is neglected, as the advective exchange processes dominate within a dual permeable medium on a regional scale.

SIMULATIONS

For first investigations the double continuum approach was applied to a fractured porous sandstone formation, considering advective transport in the fractures as well as in the matrix. The aim was to describe the regional flow and transport regime of this formation as precisely as possible. As there was no possibility to obtain the detailed information of the fracture geometry and hydraulic properties by field exploration, a reference system with known properties had to be defined. This reference system, an idealized synthetic fractured aquifer, has been used to validate the double continuum model. It is also necessary to determine physical meaningful effective parameters depending on the fracture network and rock matrix characteristics for each continuum.

Discrete reference system

For the numerical investigations of flow and transport on the synthetic fracture matrix system, the program package ROCKFLOW (Wollrath & Helmig, 1991) was used, which is based on the finite element method. A saturated two-dimensional regular fracture network was set up, where the fractures were embedded as one-dimensional line elements in a two-dimensional permeable matrix (Fig. 2(a)). This fractured porous medium contained two sets of fracture populations each consisting of 11 infinite fractures. The fractures of each population were equidistant and possessed constant aperture values of 0.001 m. The porous matrix blocks between them were defined as homogeneous and isotropic. On the in- and outflow boundary of the model Dirichlet boundary conditions were applied, which led to a constant hydraulic gradient of 5%. The other two sides of the model were no-flow boundaries. Sinks and sources were not taken into account. For transport investigations the parameters of Table 1 were applied to the system.

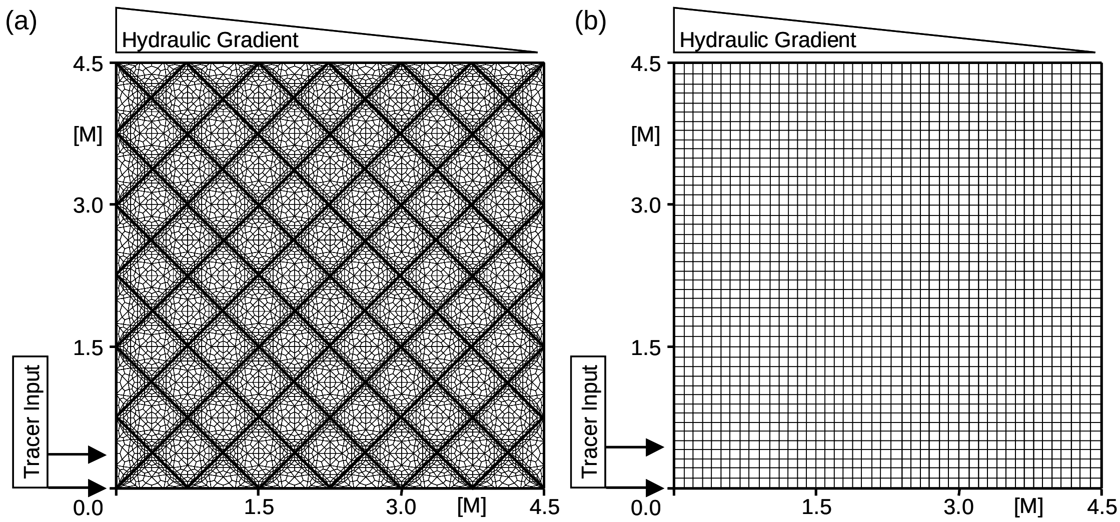

Fig. 2 Discrete (a) and double continuum (b) model set-up.

Table 1 Parameter of the discrete and double continuum system.

Parameter	Discrete system: matrix	fracture	Double continuum system: matrix	Fracture
Porosity (–)	0.1	1	0.1	0.00377
Hydraulic conductivity (m s^{-1})	10^{-6}	0.01	10^{-6}	1.84×10^{-5}
Diffusion coefficient (m^2 s^{-1})	10^{-10}	0	10^{-10}	0
Dispersivities (m)	$\alpha_l = 0.01$ $\alpha_t = 0.001$	$\alpha_l = 0.01$ $\alpha_t = 0$	$\alpha_l = 0.01$ $\alpha_t = 0.001$	$\alpha_l = 0.006$ $\alpha_t = 0.196$
Hydraulic gradient (%)	5	5	5	5
Specific exchange cross section (m^2 m^{-3})	–	–	2.0	2.0

Double continuum model

For the double continuum approach, the same geometry of the model domain was used. The discretization of the model was 45 rows, 45 columns and 1 layer, as the cells had to be small enough to account for an adequate plume reproduction (Fig. 2(b)). The boundary conditions of the double continuum model were the same as in the discrete model. The aquifer parameters of the matrix continuum were directly taken from the discrete model (Table 1). For the fracture continuum, the aquifer parameters had to be determined by inverse modelling, to reproduce the same flow and transport behaviour as given by the discrete model results. In particular, the hydraulic conductivity and the dispersion coefficients had to be determined.

RESULTS ANALYSIS

Due to symmetry only half of the plume in the longitudinal direction was simulated, to save computational effort. Therefore, the tracer was added as a point source at the margin of the inflow cross section. Figure 3 shows the resulting tracer plume of the double continuum model compared with the tracer plume of the discrete model. It can be seen, that the general shapes of the developed plumes are similar. The strong spreading of the plume in the double continuum simulation in a transverse direction could only be achieved by using a ten times higher transversal than longitudinal dispersion coefficient. This high value results due to the fact that the geometry of the fracture network has a very strong influence. The larger the angle between the fracture direction and the regional hydraulic gradient, the stronger is the transversal dispersion.

The only obvious difference between the tracer plumes in Fig. 3 is the sharp delineation to the unloaded water (c = 0 mg l^{-1}) of the discrete model due to the fracture network geometry. Even though the double continuum approach is an averaging method, which can not account for fractures in detail, the solution achieved shows a good match in comparison to the discrete one.

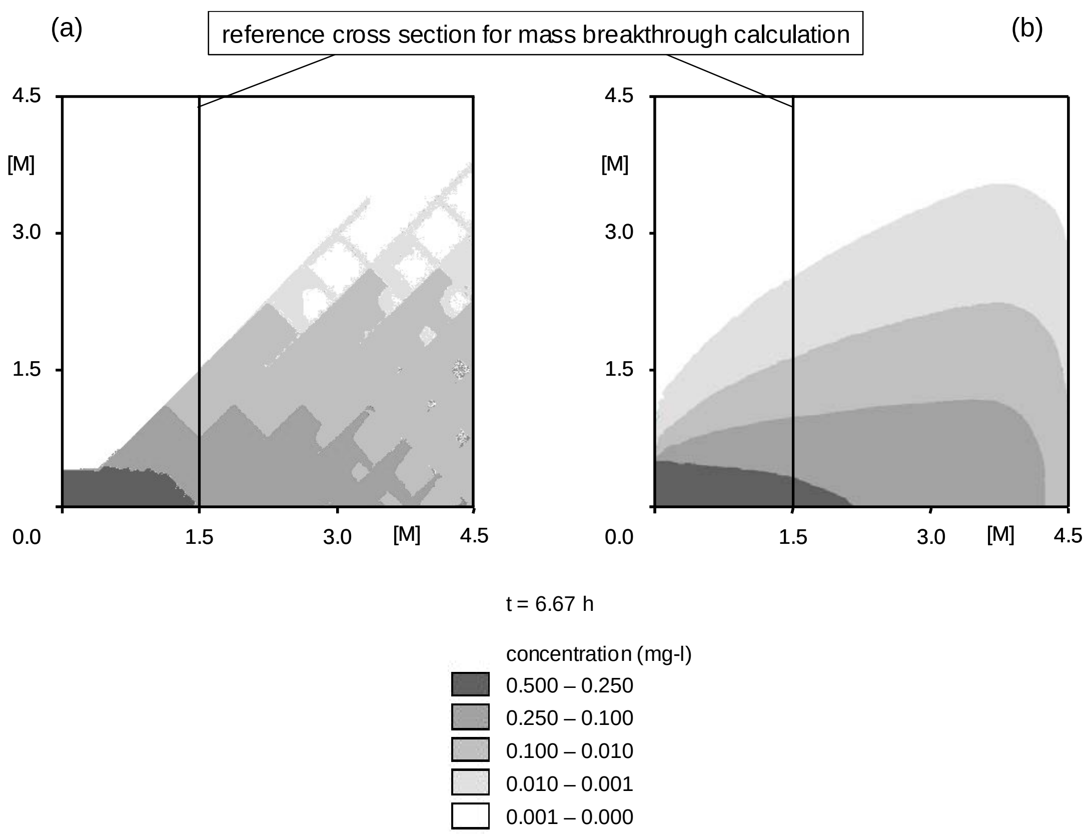

Fig. 3 Comparison of the tracer plumes after 6.67 hours of the discrete (a) and double continuum (b) model.

The reference cross section at 1.5 m in the flow direction (Fig. 3) was used to compare the relative mass breakthrough of both systems. The two results match very well (Fig. 4). This implies that the effective hydraulic conductivity as well as the longitudinal dispersion have been determined within a proper range. Both graphs show a fast tracer breakthrough and a strong tailing effect due to the fracture matrix exchange.

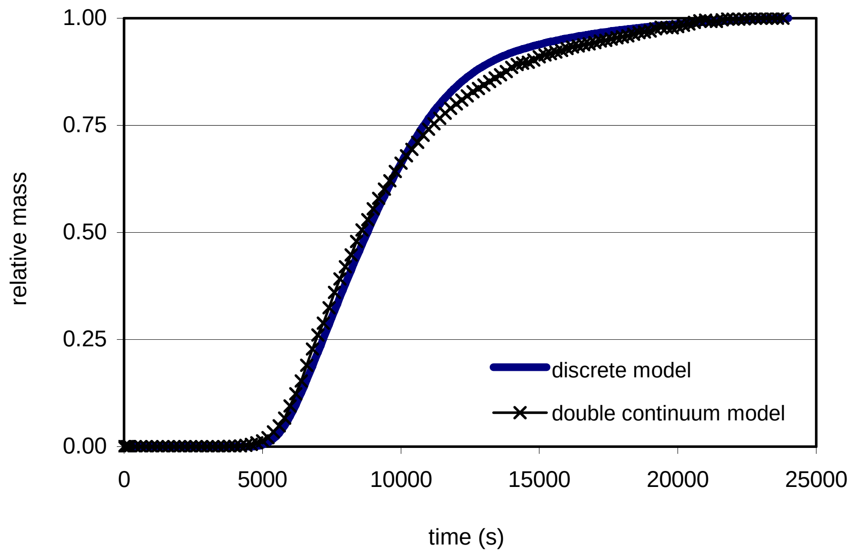

Fig. 4 Relative mass breakthrough of the discrete- and double continuum model.

CONCLUSIONS

As shown in the results analysis, the determination of the parameters for the fracture continuum is the most important step in calibrating the double continuum model and for predicting the plume development. Of particular interest is the determination of transport parameters by fracture network characteristics. For instance, the transversal dispersion coefficient and hydraulic conductivity are directly dependent on the angle between the fracture direction and the hydraulic gradient. The higher the angle, the higher is the transversal dispersion coefficient and the lower will be the resulting effective hydraulic conductivity. An increasing fracture density decreases the transversal dispersion.

By inverse modelling, these correlations in the dependence on different angles between the fractures, varying fracture spaces or heterogeneous fracture networks, have to be investigated and quantified, to enable the parameters of a fracture matrix system to be related directly to the corresponding double continuum model. Therefore the relationship between the geometric, hydraulic and transport parameters needs to be identified by detailed analyses of the calibration parameters. Also, the discretization of the double continuum model domain in comparison to the averaged matrix block size is of particular interest.

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