NUMERICAL COMPARISON OF CONCEPTUALLY DIFFERENT MODELS FOR FLOW AND TRANSPORT IN FRACTURED POROUS MEDIA

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SUMMARY

The importance of the flow and transport processes through fractured porous media has influenced development of different numerical models to predict the outcome of these phenomena. This paper compares three different models for modelling of flow and solute transport in fractured porous media, in terms of their predictions of the flow and solute transport field variables: the equivalent continuum (EC) model, the dual porosity (DP) model and the discrete fracture/non-homogeneous (NH) model. Though it is clear that the three models are based on different assumptions for their validity, it is not clear in which cases two or all of them would give similar results, since there are no such reported comparisons in the open literature. The Boundary Element Dual Reciprocity Method – Multi Domain scheme (BE DRM-MD) has been used and its implementation has been described. This numerical scheme has been used for the first time to solve a dual-porosity model. The scheme showed satisfactory accuracy and high flexibility in preparation of the discrete fracture/non-homogeneous meshes.

Key words: fractured porous media; equivalent continuum model; dual porosity model; discrete fracture model; model comparison; boundary elements

1. INTRODUCTION

With the increased demand of water all over the world, the quality problem becomes the limiting factor in the development and use of water resources. Although it may seem that groundwater is more protected than surface water, it is still subjected to pollution, and when the latter occurs, the restoration to the original, unpolluted state, is usually more difficult and time-consuming process. Therefore, the interest in the mathematical and numerical treatment of fluid flow and transport in porous media, i.e. the necessity for sophisticated mathematical models and numerical tools capable of understanding, predicting and optimising all the physical phenomena occurring in this field, has been increasingly rising.

Understanding flow and transport processes in naturally fractured porous media is of interest in environmental engineering applications, in geohydrology or in oil reservoirs engineering, when porous strata are made of rocks, which are crossed by networks of fissures and cracks. Recently, fractured rocks attracted the attention in connection with the problem of geological isolation of radioactive waste.

2. MODELING FLOW AND TRANSPORT IN FRACTURED POROUS MEDIA

Porous media often exhibit a variety of heterogeneities, such as fractures, fissures, cracks, and macro pores or inter-aggregate pores. The crystalline bedrock consists of solid rock, cut by a network of fractures. Water flows unevenly through an intricate network of paths formed by fracture intersections. However, water does not move along all of the fractures. For various reasons, no driving force exists in a number of fractures that are "dead-ends", but only in small parts, i.e. flow channels, of the fractures, which form the active flow paths with high permeability. Thus, water flows primarily along a small portion of inter-connected fractures (water-bearing fractures), while most of the fractures and other volumes with low fracture density (matrix blocks) contain essentially stagnant water. The hydraulic characteristics of the rock are mainly defined by the properties of the fracture network, i.e. the permeability, density, size and orientation distributions of the fractures.

The microscopic structures or processes affect water and solute movement at the macroscopic level by creating non-uniform flow fields with widely different velocities. Therefore, when modelling groundwater flow, the characteristics of the porous media need to be considered. From a conceptual point of view, various models can be adopted to carry out the study of water flow in the far field [1]. The type of results aimed for, the data available, the scale of the modelled volume and some practical limitations like computational resources affect the selection of the modelling approach. Furthermore, the applicability of alternative methods for modelling various physical processes in a domain is different. In the groundwater flow analyses, the fractured porous media in the far field (Fig.1a) can be modelled conceptually with three alternative approaches: *the discrete fracture models (non-homogeneous NH),* (Fig.1b), the *double-porosity (DP) models* (Fig. 1c) and the *equivalent-continuum (EC) models* (Fig. 1d).
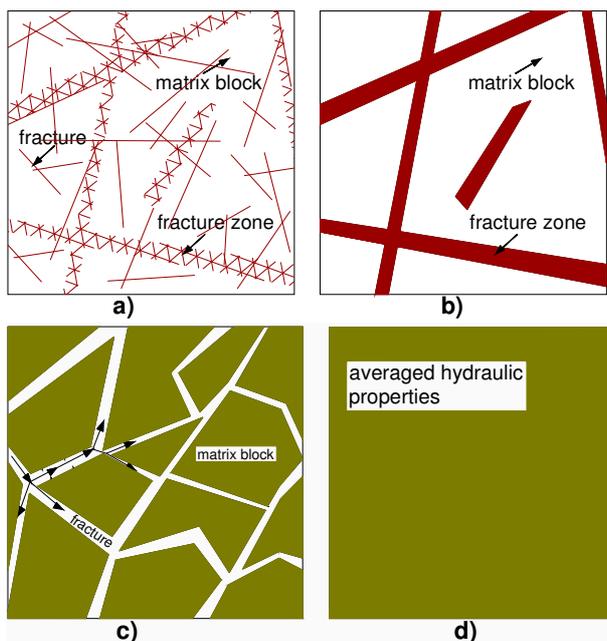

Fig. 1 a) fractured porous media; b) non-homogeneous representation; c) double porosity representation; d)equivalent continuum representation

2.1 The non-homogeneous (discrete fracture) model

The porosity and permeability for the non-homogeneous model are allowed to vary discontinuously and rapidly, as both quantities are significantly greater in the fractures than in the porous rock. Computational and data requirements for treating such a model are too large, which makes this approach not suitable for practical purposes. Therefore, it is suitable for those situations where only several fractures or fracture zones are of significance. For systems with large number of fractures the NH model becomes impractical because of the large CPU and data storage demands, see [4].

The equation that describes the transient case of saturated flow in isotropic porous media can be written as:

$$C \cdot \frac{\partial h}{\partial t} + S_{ource} = K \cdot \nabla^2 h \qquad (1)$$

where C - specific storativity [L^{-1}], h- the hydraulic head [L], K - the hydraulic conductivity [LT^{-1}], t - time [T] and S_{ource} - the source term [T^{-1}].

Equation (1) is valid for both, porous matrix and fractures. The matrix–fracture interface is treated in the same way as in any other case of non-homogeneous medium. The flow velocity field is described by the Darcy law:

$$V = -K\nabla h \qquad (2)$$

The following equation for transient solute transport is used:

$$R \frac{\partial c}{\partial t} = \frac{\partial}{\partial x_j}\left(D_{ij}\frac{\partial c}{\partial x_i}\right) - v_i \frac{\partial c}{\partial x_i} - \Omega c \qquad (3)$$

where c – solute concentration [ML^{-3}]; R – retardation factor; Ω – coefficient related to a first-order chemical reaction [T^{-1}]; v_i –velocity in the x and y direction [LT^{-1}]; D_{ij} – dispersion coefficient [L^2/T].

The first term on the right – hand side of the equation (3) describes the influence of the dispersion on the concentration distribution; the second term is the change of the concentration due to advective transport, while the third one represents concentration changes due to decay and chemical reactions.

2.2 Equivalent-continuum model

In the equivalent-continuum (EC) approach, the same equations as for the NH model, (1) and (2) for flow and (3) for solute transport, are used. The difference from the NH model is that the fractures are not modelled explicitly, the fractured bedrock is treated as a continuum. No distinction is made between the water-bearing fractures and the matrix blocks, water is assumed to flow through the whole system. The hydraulic properties of the domain are averaged over the sub-volume, or representative elementary volume

(REV), containing sufficiently large number of fractures, each hydraulic unit separately is treated as a homogeneous and isotropic continuum. They are estimated according to the equations for the simplest case of flow through domain intersected by a family of parallel fractures of equal aperture:

- for porosity

$$n_{equi} = n_m \cdot \frac{V_m}{V_t} + n_f \cdot \frac{V_f}{V_t} \qquad (4)$$

- for hydraulic conductivity

$$K_{equi} = \frac{\rho g}{\mu L}\left(\frac{mb^3}{12} + K_m(L - mb)\right)$$

$$\approx K_m \frac{V_m}{V_t} + K_f \frac{V_f}{V_t} \qquad (5)$$

where n_f and n_m - porosities of the fractures and matrix blocks in the REV, respectively, V_f and V_m - volumes of the fractures and matrix blocks in the REV [L^3], respectively, V_t - total volume of the domain [L^3], L - total thickness of the domain [L], b - aperture of the fracture [L], m - number of parallel fractures, ρ – fluid's density [mL^{-3}], μ - dynamic viscosity [$mL^{-1}T^{-1}$], and K_f and K_m - hydraulic conductivities of the fractures and matrix blocks, respectively [LT^{-1}].

The equivalent dispersion coefficient is calculated according to the following expression

$$D_{equi} = D_m \frac{V_m}{V_t} + D_f \frac{V_f}{V_t} \qquad (6)$$

where D_f, D_m are dispersion coefficients in the fractures and matrix blocks [L^2/t], respectively. The calculation of the equivalent dispersion coefficient is obtained under assumption of parallel fractures and flow parallel to the fractures, and steady state condition when there is no more lateral diffusion into the matrix. Under such conditions the transport is also parallel to the fractures and the 2D problem is reduced to a 1D problem, both in the fractures and porous matrix, and the following equation is used for the respective dispersion coefficients:

$$D_{x(i)} = a_{L(i)}V_{x(i)} + D_{d(i)} \qquad (7)$$

where a_L - longitudinal dispersivity, D_d - the coefficient of molecular diffusion, and (i) stands for m, matrix block, or f, fracture.

Although the EC model is commonly employed in describing fractured bedrock, there are some problems associated with it. The results obtained with the EC model represent averaged values over sufficiently large

volumes of the domain, and therefore it is impossible to have a reliable estimate of the hydraulic head or concentration in a certain point of the domain.

2.3 Dual porosity model

As an alternative, discontinuous nature of the porosity and permeability can be avoided by replacing them locally by their average values, and the interchange between the fracture and the matrix must be modelled. In such a model, the void space of the fractures is visualized as a continuum (occupied by one or more fluids), while the void space within the blocks is regarded as another continuum that is occupied by the same fluid, or fluids, see [6], [7], [8]. The two void-space continua may exchange fluid's (or fluids') mass between them at every macroscopic point within the considered domain. The transport of other extensive quantities, e.g. mass of the solute, may also take place within each of the two continua, with a possible exchange between them.

Double porosity (DP) model is much more complicated mainly from the fact that since the fracture system is viewed as a porous medium, both matrix and fracture flow and transport are defined at each point of the matrix. The numerical double-porosity model assumes that the equation for transient water flow and the convection-dispersion equation for solute transport can be applied to both pore systems. Hence, macroscopically, two flow velocities, two pressure heads, two water contents and two solute concentrations characterize the porous medium at any point in time and space. The model assumes that the properties of the bulk porous medium can be characterized by two sets of local-scale properties: one set associated with the fracture pore system (subscript f) and the other with the matrix pore system (subscript m).

Assuming applicability of Darcy's law, saturated water flow in the fracture and matrix pore regions are described by a coupled pair of equations [7],[8]:

$$\nabla^2 h_f = \frac{C_f}{K_f}\frac{\partial h_f}{\partial t} + \frac{\alpha_w(h_f - h_m)}{w_f K_f} \qquad (8.1)$$

$$\nabla^2 h_m = \frac{C_m}{K_m}\frac{\partial h_m}{\partial t} + \frac{\alpha_w(h_m - h_f)}{w_m K_m} \qquad (8.2)$$

where: h – pressure head [L]; C – specific water capacity dθ/dh [L^{-1}]; K – hydraulic conductivity [LT^{-1}]; t – time [T]; w_f – relative volumetric proportion of the fracture pore system; $w_m = 1 - w_f$;

$\Gamma_w = \alpha_w \left(h_f - h_m \right)$ – water transfer term [T^{-1}]   (9)

$\alpha_w = \alpha_w^* \cdot K_a = \dfrac{\beta}{a^2} \gamma_w K_a(u)$ – first-order mass

transfer coefficient for flow [L^{-1}T^{-1}]   (10)

a - distance (L) from the centre of the fictitious matrix block to the fracture boundary (half width of the matrix block); β – dimensionless factor depending on the geometry of the aggregates, β =3 (for rectangular slabs) – 15 (for spheres); γ_w = 0.4 (more or less independent of the aggregate geometry and the applied initial pressure and conditions); K_a – effective hydraulic conductivity of the matrix at the fracture/matrix interface.

In the similar manner as for the flow, the solute transport in a saturated fractured porous medium is described using two coupled double-porosity advection-dispersion equations, here directly written as non-homogeneous Laplace equations for the sake of brief presentation:

$$\nabla^2 c_f = \frac{1}{D_f} \left(R_f \frac{\partial c_f}{\partial t} + v_{f_i} \frac{\partial c_f}{\partial x_i} + \Omega_f c_f + \frac{\Gamma_s}{w_f} \right)$$

$$\nabla^2 c_m = \frac{1}{D_m} \left(R_m \frac{\partial c_m}{\partial t} + v_{m_i} \frac{\partial c_m}{\partial x_i} + \Omega_m c_m - \frac{\Gamma_s}{w_m} \right) \quad (11)$$

3. NUMERICAL IMPLEMENTATION

In spite of the large number of existing numerical packages for simulation of the fluid flow and contaminants transport in fractured porous media, most of them are based on the Finite Element (FEM) and Finite Difference (FDM) methods. Here, the Boundary Element Dual Reciprocity Method – Multi Domain scheme (BE DRM-MD) has been used and implemented. The general idea of the BEM is to transform the original partial differential equation (PDE), or set of PDEs that define a given physical problem, into an equivalent integral equation (or system) by means of the corresponding Green's theorem and its fundamental solution [12], [13]. In this way some or all of the field variables and their derivatives are necessary to be defined only on the boundary. The governing equation that describes a linear time-dependent process of flow and transport in the models, in the general form can be written as,

$$\nabla^2 u = b\left(x, y, u, t \right) \text{ in the domain } D \quad (12)$$

with the: 'essential' or Dirichlet boundary conditions of the type $u = \bar{u}$ on Γ_1; 'natural' or Neumann boundary conditions $q = \partial u / \partial n = \bar{q}$ on Γ_2; eventually, 'mixed' or Robin boundary conditions of type $au + b\dfrac{\partial u}{\partial n} = c$
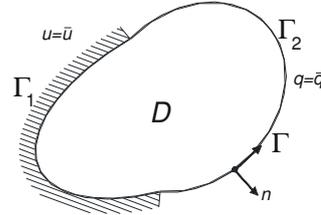

Fig.2. Definition of domain with boundary conditions

Here $\Gamma = \Gamma_1 + \Gamma_2$ is the exterior boundary that encloses the domain D and n is its outward normal, see Fig. 2.

For the non-homogeneous and the equivalent continuum models u represents $h(x_i,t)$ in the equation (1) for the flow and $b = \dfrac{1}{K} \left(S_{ource} + C \dfrac{\partial h}{\partial t} \right)$, while for the transport equation (3), $u \equiv c(x_i,t)$ and $b = \dfrac{1}{D} \left(v_i \dfrac{\partial c}{\partial x_i} + \Omega c + R \dfrac{\partial c}{\partial t} \right)$. For the double porosity model, according to the governing equations for the flow (8), $b = \dfrac{1}{K_f} \left(C_f \dfrac{\partial h_f}{\partial t} + \dfrac{\Gamma_w}{w_f} \right)$ and according to the governing equations for the transport (11), $b = \dfrac{1}{D_f} \left(R_f \dfrac{\partial c_f}{\partial t} + v_{f_i} \dfrac{\partial c_f}{\partial x_i} + \Omega_f c_f + \dfrac{\Gamma_s}{w_f} \right)$.

The above expressions are for the fracture system, and similar ones are defined for the matrix blocks.
Applying the DRM-MD approach to the equation (12), according the detailed explanation in references [14], [15], yields:

$$\boldsymbol{H}_i \boldsymbol{u} - \boldsymbol{G}_i \boldsymbol{q} = (\boldsymbol{H}_i \hat{\boldsymbol{u}} - \boldsymbol{G}_i \hat{\boldsymbol{q}}) \boldsymbol{F}_i^{-1} \boldsymbol{b} \quad (13)$$

The two boundary element characteristic matrices H and G on both sides of the equation (13) are consisted of coefficients, which are calculated assuming the fundamental solution is applied at each node successively, and depending only on geometrical data, see [12]-[14].

A code that offers high flexibility in mesh generation, which can be built of sub-domains of various sizes, geometries and numbers of boundary elements per sub-domain, was developed.

4. NUMERICAL TESTS OF THREE SCHEMES

Before any case studies were analysed, verification of the numerical approach was performed for both, flow and transport equations. Once the accuracy of the basic BE DRM-MD scheme was verified, a number of transient cases for flow and solute transport were solved using the EC, NH and DP models.

4.1 Flux calculation procedures for the models

The total flow and transport fluxes through the fractured porous domain are compared in different examples. The water fluxes for different models are calculated using the following equations:

▪ For the EC model: $\phi = -K \dfrac{\partial h}{\partial n} b$ (14)

▪ For the NH model:

$$\phi_f = -\sum_{i=1}^{k} K_{fi} \frac{\partial h_{fi}}{\partial n_i} b_{fi} \text{ - for the fractures}$$ (15a)

$$\phi_{mb} = -\sum_{j=1}^{k} K_{mbj} \frac{\partial h_{mbj}}{\partial n_j} b_{mbj} \text{ - matrix blocks}$$ (15b)

$$\phi_{total} = \phi_f + \phi_{mb}$$ (15c)

▪ For the DP model based on volumetric factor w_f:

$$\phi_f = -K_f \frac{\partial h_f}{\partial n} w_f b \text{ - fractures}$$ (16a)

$$\phi_{mb} = -K_{mb} \frac{\partial h_{mb}}{\partial n} (1 - w_f) b \text{ - matrix blocks}$$ (16b)

or based on the total fracture aperture taking part in the considered domain cross section

$$\phi_f = -K_f \frac{\partial h_f}{\partial n} b_f \text{ - fractures}$$ (17a)

$$\phi_{mb} = -K_{mb} \frac{\partial h_{mb}}{\partial n} b_{mb} \text{ - matrix blocks}$$ (17b)

$$\phi_{total} = \phi_f + \phi_{mb}$$ (17c)

where: ϕ_f - total flow flux in the fractures for the considered cross section; ϕ_{mb} - total flow flux in the matrix block for the considered cross section; ϕ_{total} - total flow flux for the considered cross section; w_f - relative volumetric proportion of the fracture pore

system; K_f , K_{mb} -hydraulic conductivities for the fractures and matrix blocks, respectively; $\dfrac{\partial h_f}{\partial n}, \dfrac{\partial h_{mb}}{\partial n}$ - normal derivatives to the cross section in the fractures and matrix blocks, respectively; b - total width of the domain; b_{fi} - aperture of one fracture; b_{mj} - width of a single matrix block; b_f - total aperture of fractures through the cross section, $\left(b_f = \sum_{i=1}^{k} b_{fi} \right)$; b_{mb} - total aperture of matrix blocks through the cross section, $\left(b_{mb} = \sum_{j=1}^{m} b_{mbj} \right)$; k - number of fractures in the considered section; m - a number of matrix blocks in the considered section.

Note that Eqs. (16) and (17) differ since Eq. (16) uses the volumetric factor w_f, which includes fractures with active and stagnant flow, in calculation of the fluxes, while Eq. (17) uses just the aperture of the active/water-bearing fractures, or the ones that form part of the considered cross section through which the flux is calculated. It is also important to note that in a general case b_f and b_{mb} will differ from w_f and $(1- w_f)b$, respectively. The solute fluxes are calculated in a similar way as the water fluxes.

4.2 Example

In this example, a square area of dimensions 0.46 x 0.46 with six fracture zones intersecting under 90° angle is analysed, see Fig.3. Two different geometrical distributions of fractures were analysed. The first one has two arrays of fractures, one parallel to the flow and one perpendicular to the flow, see Fig. 3a), in this example referred to as the "original" fracture network, and the other one is "rotated" for an angle of 45° in respect to the original geometry/fracture network, Fig.3b). In both cases the analysed areas of the domains, the mutual distance between fractures and the volumetric factor of the fractures are equivalent. The purpose for analysing these two orientations of the fracture networks was to establish the sensitivity of the NH model, as a reference model towards which the other two are compared, to the orientation of the fracture network in respect to the direction of the flow. This information is important since the other two selected models, being isotropic, cannot take into account the orientation of the fracture network in respect to the direction of the flow.

a) original fracture network   b) rotated fracture network

discretisation 1: nc=49; ngn=64   discretisation 3: nc=65; ngn=84

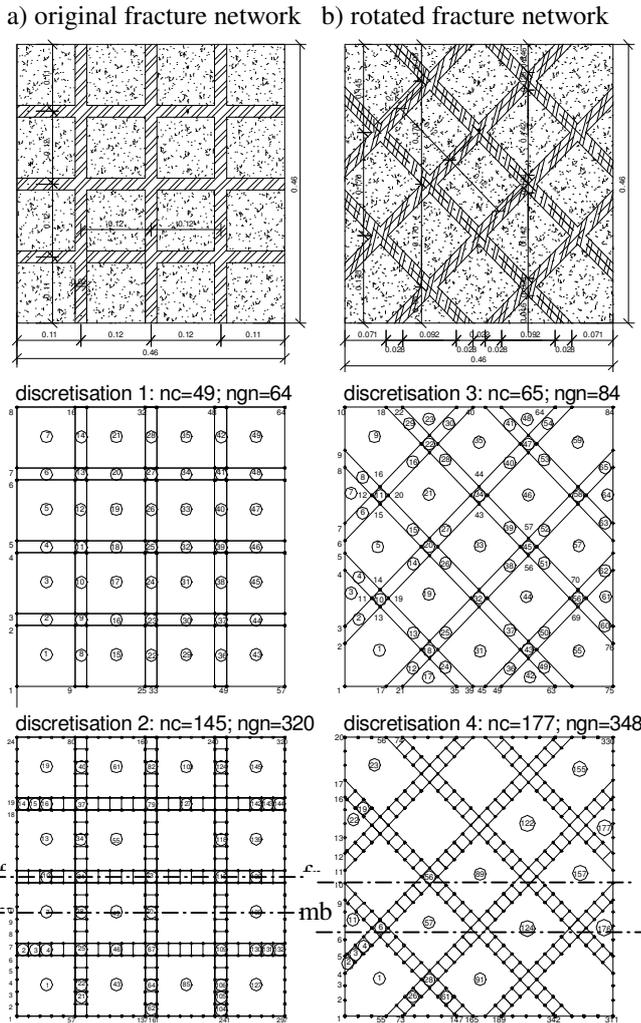discretisation 2: nc=145; ngn=320   discretisation 4: nc=177; ngn=348

Fig. 3: Square mesh with discrete fracture zones:
a) original fracture network with two discretizations;
b) rotated fracture network with two discretizations

According to Fig. 3a), the double porosity model was designed with all the necessary design parameters, which include the half-distance between the fractures $a = 0.06$m, volumetric factor $w_f = 24.4\%$, geometry of the matrix blocks $\beta = 3.0$, $\gamma_w = 0.4$, and effective hydraulic conductivity Ka is taken as an average value of both conductivities in the matrix block $K_m = 8.64 \times 10^{-5}$m/d, and in the fractures $K_f = 8.64 \times 10^{-3}$m/d. The value of the specific storativity used for all the models is 10^{-4}m^{-1}. Dispersion coefficients $D_f = 0.05$m^2/d and $D_m = 0.005$ m^2/d were used for the transport simulation. The equivalent properties for the EC model were calculated using Eqs. (5) and (6).

Boundary conditions prescribed for the fluid flow are: $h_f(0, y, t) = h_m(0, y, t) = 1.05$m at the inlet surface and $h_f(L, y, t) = h_m(L, y, t) = 1.0$m at the outlet surface, $q_f(x, 0, t)$, $q_m(x, 0, t)$ and $q_f(x, b, t)$, $q_m(x, b, t)$

The flow field is with a hydraulic gradient of 5%. Boundary conditions prescribed for the transport simulation are: $c_f(0, y, t) = c_m(0, y, t) = 1.2$ at the inlet surface and $c_f(L, y, t) = c_m(L, y, t) = 1.0$ at the outlet surface. At $y = 0$ and $y = b$, a zero normal derivative boundary condition is imposed, (impermeable boundary). Here, L is the length of the adequate domain and b is its width.

Initial conditions in the fracture and the matrix pore system are: $h(x, y, 0) = 1.0$m for the flow and $c(x, y, 0) = 1.0$ for the transport.
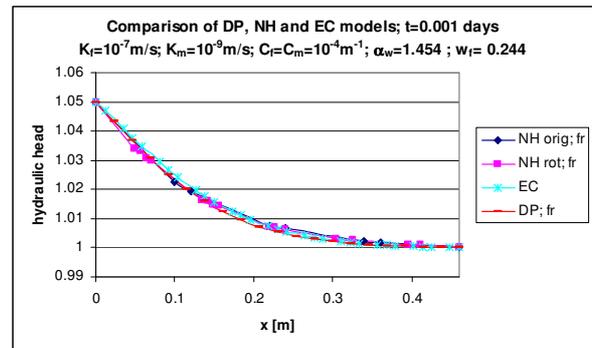

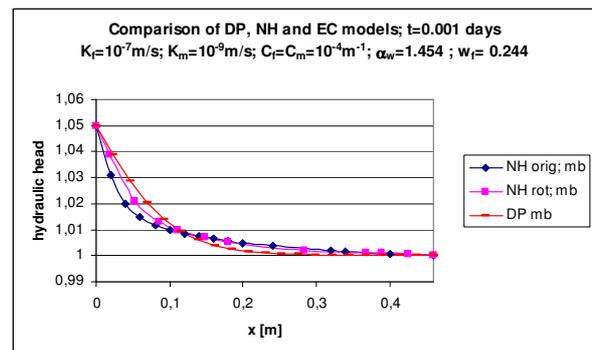Fig.4: Hydraulic head profiles for the fractures estimated using three models; t=0.001days

Fig.5: Hydraulic head profiles for the matrix blocks using three models; t=0.001days

For the NH model for the first mesh with horizontal and vertical fractures, two discretizations were made: one using 49 sub-domains and 64 geometrical nodes and the second one with 145 sub-domains and 320 nodes. Numerical simulations for both of the fracture networks were virtually identical and nodal values for the

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hydraulic heads and concentrations differ only after the fourth significant digit. The maximum discrepancies are about 0.01%.

Small differences in computed hydraulic heads indicate clearly that the domain discretization is fine enough for the present example to obtain an accurate numerical solution using the NH model. The analyses showed that for heterogeneous systems like this there is no need of extremely fine meshes. Meshes used for the DP and EC models were built of 100 equal square sub-domains.

Fig.4 shows the comparison of results for hydraulic head profiles in the fractures for $t = 0.001$ days obtained using the three models. The profile fr in the NH model with "original" fracture network is taken in the middle fracture, y=0.235m, while the profile in the matrix blocks mb is taken at y=0.175m, see Fig. 3. The profile fr for fracture in the NH model with the "rotated" network follows the flow in the "zigzag" way of the fracture. Note that the EC model has only one solution. The results obtained with the three models are in good agreement. In Fig. 5 the comparison of hydraulic heads in the matrix block for $t = 0.001$ days obtained using the DP and NH models is shown. The agreement is better between the results obtained using the NH model with two different fracture networks, while the DP model shows a bit larger discrepancy. Since the flow is much faster in the fractures, and therefore of more significance, the agreement between the models for estimated hydraulic heads can still be considered to be satisfactory. Actually, as $t \to \infty$, when the models reach steady state, both DP (the fractures, as well as the matrix blocks) and EC models have linear hydraulic heads, see Fig. 6, or their solutions are one-dimensional and equal, while the NH model has two-dimensional solution which is also confirmed with the existence of the transversal velocity v_y, see Fig. 8.
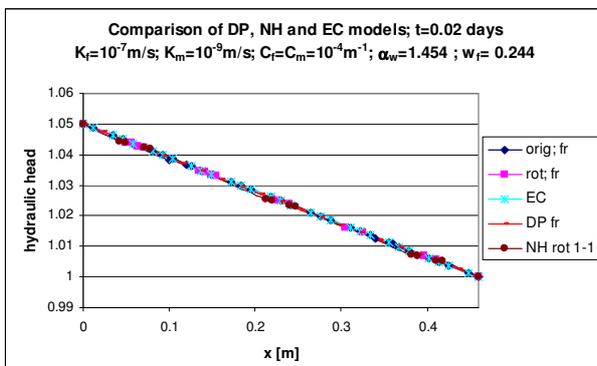

Fig. 6a: Hydraulic head profiles for the fractures using three models; t=0.01days

Although it may seem that all the lines are linear and overlapping one each other, still there is a difference in the behaviour of the three models. Namely, the EC and DP (both for the fractures and matrix blocks) models have linear one-dimensional solutions, while the NH model (both the "original" and the "rotated" one) have two-dimensional complex solutions. In purpose to make it obvious, the hydraulic head for the NH with "rotated" fracture network in two profiles (1-1 at y=0.1415m and 2-2 at y=0.2265) is given in separate figures, see Fig. 6b and 6c. For the NH model with the "original" fracture network happens something similar, but it is not obvious in the Figures 6 because the zones with high permeability in the horizontal profiles are not as wide as in the NH model with the "rotated" mesh.
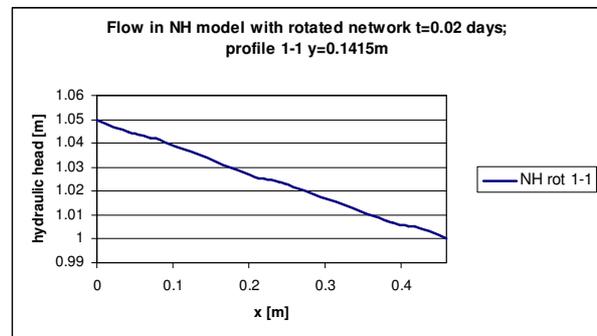

Fig. 6b: Hydraulic head profile 1-1 at y=0.1415m; NH model with rotated mesh; t=0.02d

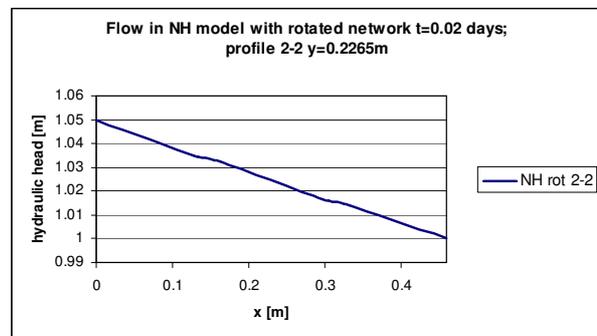
Fig. 6c: Hydraulic head profile 2-2 at y=0.2265m; NH model with rotated mesh; t=0.02d

Figures 7 and 8 show the calculated flow fields in the fractures for both NH models with "original" and "rotated" fracture networks. It can be seen that the vertical fractures, because of the type of boundary conditions used for y=0 and y=0.46, in the "original" fracture network have little influence on the flow, while in the "rotated" fracture network larger proportion of the fractures have an active role. Note that the length of the velocity vectors in the figures are automatically scaled

and may not give an accurate representation of the magnitude of the velocity vectors in the two meshes. With the Fig. 7 and 8, the complex two-dimensional solution of the NH models when the time tends to infinity and the steady state is reached ($t \rightarrow \infty$) is confirmed again.
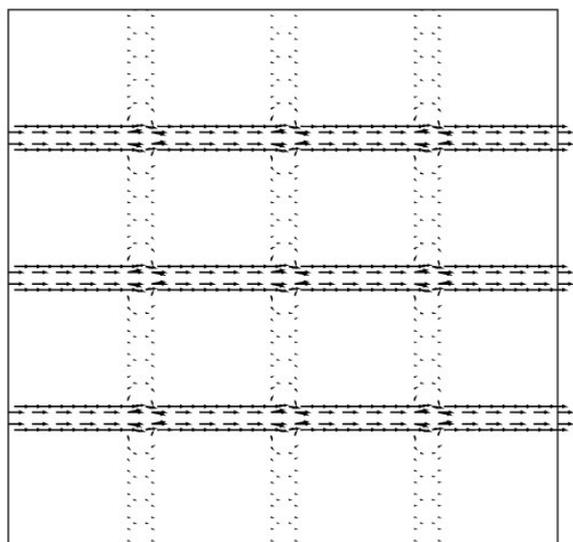

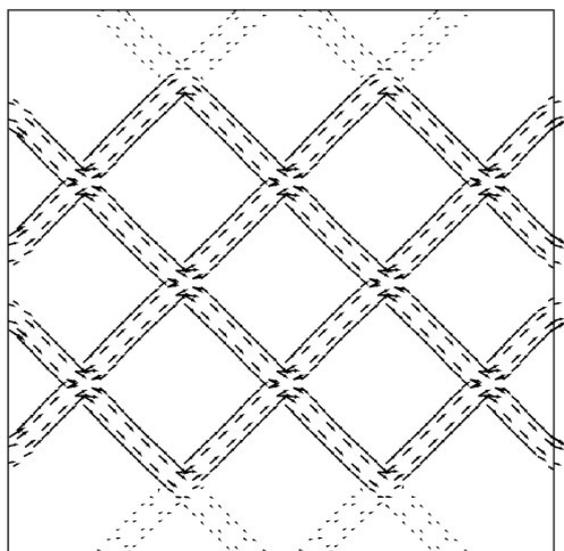Fig. 7: Velocities in the fractures for NH model with original mesh

Fig. 8: Velocities in the fractures for NH model with rotated mesh

The comparison of estimated total flow fluxes on the inlet and outlet of the domain are shown in Figures 9 and 10, respectively. The flux for the DP model was calculated in two different ways. The first estimation makes use of Eq. (16) and the volumetric factor w_f of the fractures, while the second estimation uses Eq. (17) and the exact aperture of the fractures participating in the considered cross section, i.e. detailed picture of the fracture network is needed. In the figures $DP(wf)$ refers to the approach that uses (16), and DP refers to the one that uses (17). It is apparent that both NH solutions obtained using two different meshes and the DP model using equation (17) show flux results that are in good agreement. The NH model with rotated mesh overshoots the other two solutions for the flux on the inlet in the transient period, perhaps due to the larger portion of the fractures that are actively involved in the flow, see Fig. 8.

Note that in this example the volumetric factor differs from the sum of apertures of fractures participating in the considered cross section. In the first example it did not make any difference whether the volumetric factor w_f or the exact total aperture of fractures was used to calculate the flux through the fracture network, since they were identical, because all the existing fractures were included in the flow. Using Eq. (16) in this case overestimates the total aperture of fractures effectively taking part in the flow through a given cross section.
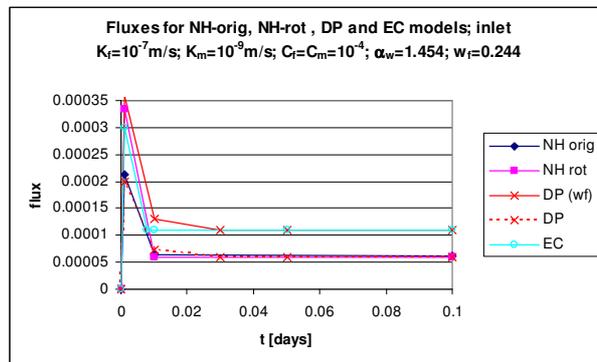

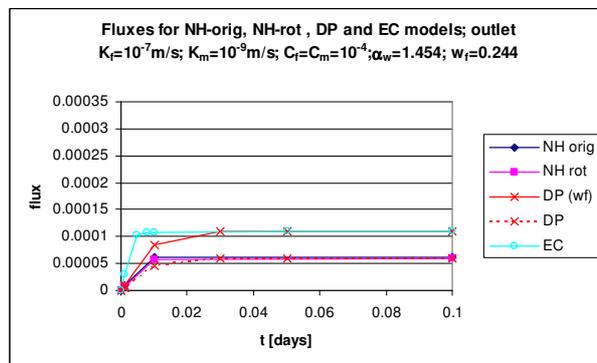Fig.9: Total flow fluxes at inlet surface for 3 models

Fig.10: Total flow fluxes at outlet surface for 3 models

This shows that when calculating the fluxes with the DP model it is not enough to know the volumetric factors only, for more accurate calculation information about the geometry and orientation of the fracture network is needed. This is in contradiction with the general idea of the DP models which consider the domain to be homogeneous.

The EC model encounters similar problems as the DP model using Eq. (16), as the equivalent hydraulic conductivity, calculated using Eq. (5), gives an overestimate due to the V_f/V_t term, which takes into account the vertical fractures that do not have significant contribution towards the flow. The accuracy of the flux estimated using the DP model can be improved using the exact aperture of the fractures in the cross section, but the accuracy of the flux estimated using the EC model adopted in this study cannot be improved since the V_f/V_t term is part of the model itself and cannot be eliminated.

The results show good agreement for the NH model with two different meshes, Figs. 5.3a) and 5.3b), indicating that the orientation of the fracture networks in respect to the direction of the flow does not influence significantly the results in this case.

Both fluxes for the DP model, Eqs. (16) and (17), show prolonged transient period, though to smaller extent than what was observed in Example 1.

Figs. 11a and 11b show the concentration profiles for t=0.5 days in the fractures and matrix blocks, respectively. Regarding the fractures, the results show slightly larger discrepancies than the results for hydraulic heads.
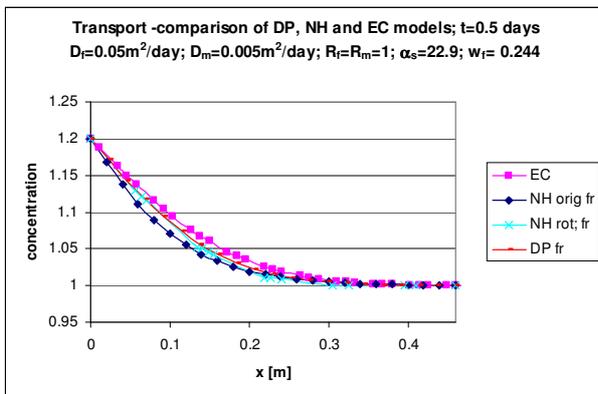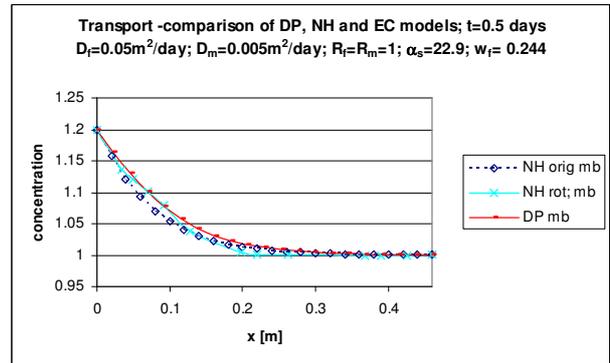

Fig. 11b: Concentration profiles for the matrix blocks for the three models; t=0.5 days

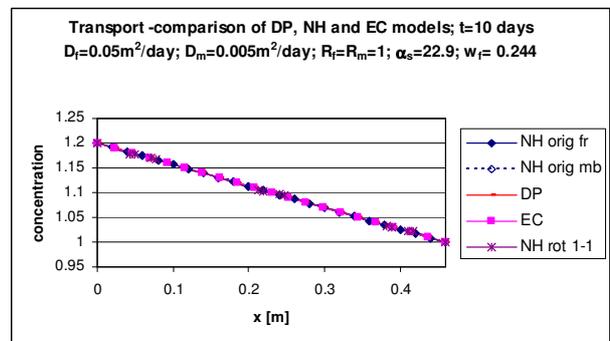Fig.12a: Concentration profiles for the matrix blocks for the three models; t=10 days

As the time progresses, the steady state is reached. In Fig. 12a the comparison is given for all three models for time t=10days. Similarly as for the flow processes, transport processes of the EC and DP models show one-dimensional solution and the NH model solution is two-dimensional.
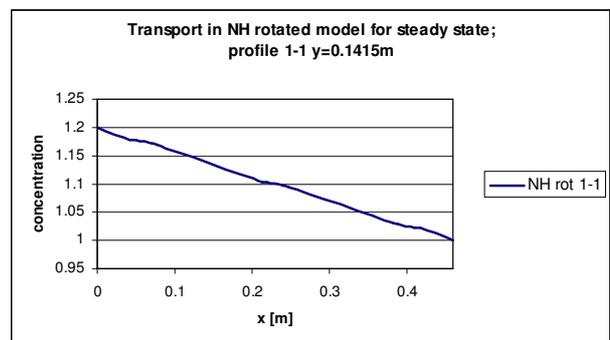

Fig. 11a: Concentration profiles for the system of fractures for the three models; t = 0.5 days

Fig. 12b: Concentration profile 1-1 at y=0.1415m; NH model with rotated mesh; t=10 days
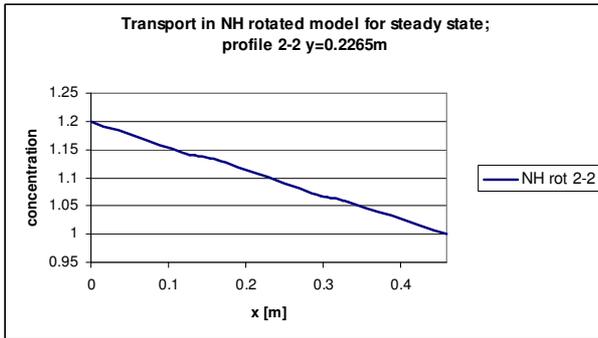
Fig. 12c: Concentration profile 2-2 at y=0.2265m; NH model with rotated mesh; t=10 days

Concentration profiles of the NH model with "rotated" fractures are extracted and given separately in the Fig. 12b and 12c in order to show the solution more obviously.

The variations in time of the total solute fluxes for the three models on the inlet and on the outlet of the domain are shown in Figs. 13 and 14, respectively. The fluxes of solute mass include an advective flux, expressing the flux carried by the water at an average velocity, and dispersive flux that produces the spreading or dispersion of the solute. Larger discrepancies are found on the inlet in the early stages of the simulation $t < 0.2$, see Fig. 13.
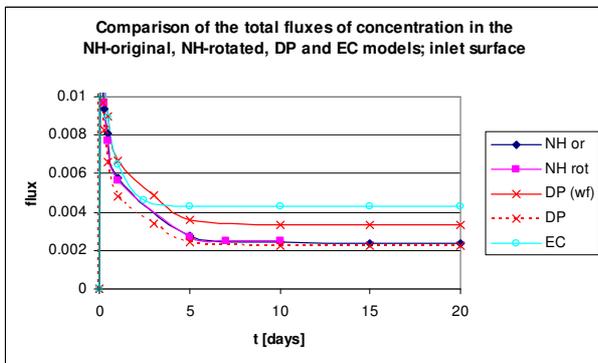

Fig. 13: Total solute fluxes for three models at the inlet

On the outlet, the total solute fluxes obtained with both NH meshes and the DP model using real fractures' apertures are in good agreement. The solute fluxes estimated with the EC model and the DP model using volumetric factor w_f show larger discrepancy from the other three estimates, for a reason similar to the one producing discrepancy for the water flux. Unlike the previous case when the water fluxes were estimated, the solute steady state fluxes are not the same for the EC

and DP model using volumetric factor, as the total flux has got two components, advective and dispersive, making these two fluxes differ more significantly. For each model the inlet flux is equal to the outlet flux in the steady state, i.e. there is no loss of the mass.
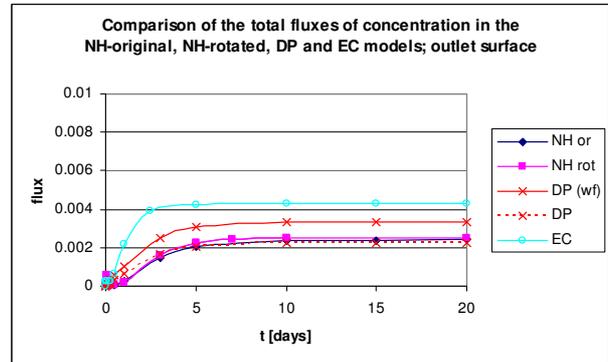

Fig. 14: Total solute fluxes for three models at the outlet

A 2D view of the isolines for the hydraulic head and concentration for the two different meshes of the NH model and for the DP model can be seen in Figures 15 and 16.
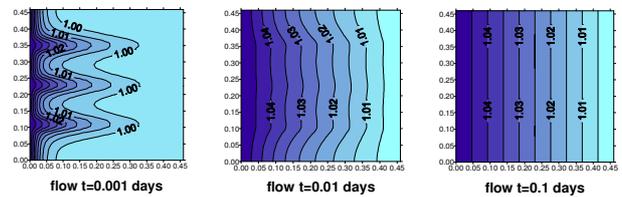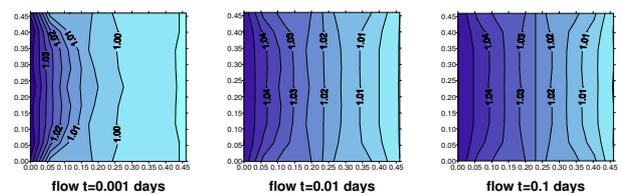

Fig.15a: Isolines for flow; NH model – original mesh
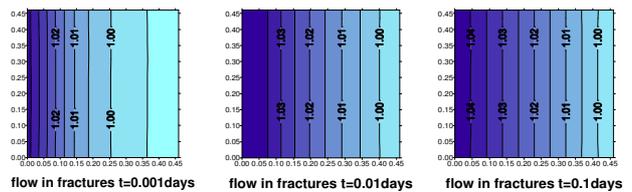

Fig.15b: Isolines for flow; NH model – rotated mesh

Fig.15c: Isolines for flow; DP model – fractures

It can be seen that for the double porosity model smooth curves occur (Fig. 15c, 16c), since the domain is observed as a homogeneous one with adequate characteristics. But for the non-homogeneous models, either with the original (Fig. 15a and 16a) or with the rotated mesh (Fig. 15b and 16b), the flow and transport are emphasised through the fractures, which is a result of the much higher permeability in the fractures, 100 times greater than in the matrix blocks. The contaminant in the DP model moves faster in the primary porosity (through the fractures), then it does in the NH models, and the amount of the pollutant in the matrix blocks remains lower. There is little advective transport in the matrix blocks for the DP model. The exchange of contaminant between a fracture and the matrix is characterised by a simplified representation of the fracture geometry and by diffusion coefficients.
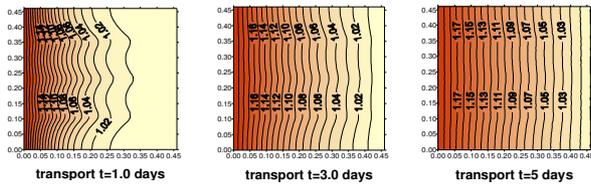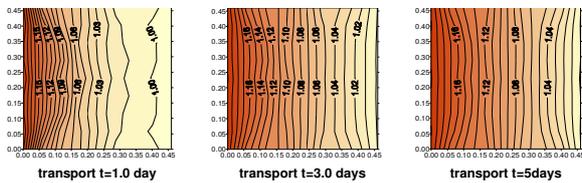

Fig.16a: Isolines for transport; NH model–original mesh

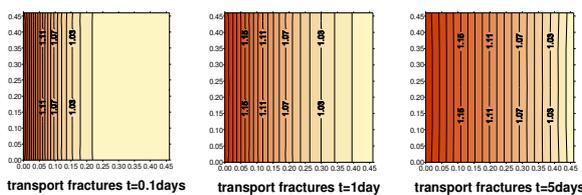
Fig.16b: Isolines for transport; NH model–rotated mesh

Fig.16c: Isolines for transport; DP model – fractures

The accuracy of the solution for the transport for the DP model is strongly affected by the accuracy of the assumed solute exchange term between fractures and matrix blocks. From that point of view, one would favour the non-homogeneous models, since they require fewer parameters. On the other hand, in spite of the averaging of the values of the hydraulic heads and solute concentrations inside the domain, the much

simpler geometrical mesh of the double porosity model offers in some instances fast and practical way of obtaining sufficient information about the flow and solute transport in the fractured porous media. The results showed that the parameters of the DP model are easy to define for uniform networks of fractures where the fractures have similar characteristics. One thing that DP model cannot provide is detailed insight in the variation of field variables inside the observed domain, especially inside and in the vicinity of large fractures.

5. CONCLUSIONS

Three different models for solving flow and solute transport in fractured porous media are compared for this study. These models are: equivalent continuum (EC), double porosity (DP) and non-homogenous /discrete fracture (NH). It is assumed that the flow and the solute transport are described by the Darcy law and the advection-dispersion equation, respectively.

▫ The advantage of the EC model is that it is the simplest one and easiest to use. It can provide good agreement for a case where the equivalent characteristics of the fractured porous media are easy to be estimated, as in case of fracture network parallel to the flow. The disadvantage of the EC model is that it cannot provide insight in the processes of flow and solute transport in the two different media, porous matrix and fractures, and would provide less accurate results when the estimation of the equivalent characteristics of the fractured porous media cannot be easily performed.

▫ Double porosity models can be used to obtain sufficiently accurate results for practical purposes, especially for modelling domains with large number of fractures with repetitive geometry and similar characteristics, not having to engage into preparation of complicated input data due to the complex geometry of the problem. The DP model offers more information than the EC model regarding the averaged properties of the flow and transport processes in the porous matrix and fractures.

▫ The sensitivity analysis of the DP model to variations of the transfer term showed that substantially different results can be obtained depending on the chosen parameters. When the transfer term α_w is smaller, or matrix blocks larger, the difference between the hydraulic heads in the fractures and the matrix blocks becomes larger. The steady state is achieved after shorter time for smaller α_w.

▫   The NH model provides the largest amount of information for the flow and transport processes of the three models that were compared and is usually seen as the most accurate, as it introduces a smaller number of assumptions /approximations than the other two models. It has been shown that the orientation of the fracture zones through the domain has little influence on the results obtained using the NH model, providing that the matrix blocks are homogenous and of uniform geometry and the fracture network consists of fractures with same properties. The disadvantage of the NH model is that the exact geometry of the fracture network is not usually known, it is difficult to prepare the meshes for complicated geometries and distributions of fractures in the porous media, and it would impose serious computational difficulties in terms of CPU and memory requirements when the number of fractures is large.

▫   The comparison of results for hydraulic heads and solute concentration showed good agreement for the three models in most of the cases. The results for water and solute fluxes showed that special care has to be taken when EC or DP models are used. The main reason for this is that for calculation of fluxes the cross sectional area must be taken into account. For the DP and NH models the total flux consists of a flux through the fractures and a flux through the matrix blocks which participate in the cross section of interest. While the NH model can accurately estimate the fluxes since the total cross section of the fractures which participate in the cross section is accurately estimated, in the case of an isotropic DP model in a general case the fluxes would be estimated by using the volumetric factor of the fractures, which introduces errors. The problem arises since not only the "active" fractures, which contribute towards the flux, are taken into account, but also the fractures with stagnant water, providing a significant overestimate of the flux. Also, the fluxes inside the fractures are normally much higher than in the matrix blocks, making the error of the fluxes in the fractures more significant when calculating the total flux.

One solution to this problem is to use more accurate estimate of the total aperture of the fractures, which participate in a given cross section, as was done in the examples. However, such approach cannot be used in the EC model, since there is only one type of porosity/permeability in this model.

The BE DRM-MD has been used for the first time to solve the double porosity model. The examples showed that this BE formulation provides stable results for grid Pe=2 and Cr=1 and can be used successfully for solving flow and transport processes in fractured porous media. The major reason why the BE DRM-MD can be attractive is that the fractures can be modelled with smaller elements/sub-domains and the matrix blocks can be modelled using single domains of various shapes and sizes, reducing the need for very fine meshes around fractures. Meshes that can easily be adapted to a considered problem have in the past been implemented using FEM – BEM hybrid methods, usually for modelling heterogeneous domains with different physical properties. The present formulation has one advantage in respect to the FEM – BEM hybrid approach, it does not have the problems related to the coupling compatibility of the two methods.

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НУМЕРИЧКА СПОРЕДБА НА КОНЦЕПТУАЛНО РАЗЛИЧНИ МОДЕЛИ ЗА ТЕК И ТРАНСПОРТ ВО ПОРОЗНИ СРЕДИНИ

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Резиме

Важноста на процесите за тек и транспорт низ порозни средини го поттикна развојот на различни нумерички модели за прогноза на резултатите од овие феномени. Во овој труд е направена споредба на три различни модели за тек на подземни води и транспорт на контаминанти: моделот за еквивалентен континуум (ЕК), двојно порозниот модел (ДП) и нехомогениот модел (НХ) со дискретни пукнатини. Иако е јасно дека трите модели се базираат врз различни претпоставки за нивната валидност, не беше јасно во кои случаи два од нив или сите три даваат слични резултати, бидејќи не постојат такви споредби во достапната литратура. Користена е Методата на гранични елементи со двоен реципроцитет - шема со мултидомени и објаснета е нејзината имплементација. Оваа нумеричка шема е за прв пат користена за решавање на моделот со двојна порозност. Таа покажа задоволителна точност и голема флексибилност во подготовката на моделите, особено на нехомогените мрежи со дискретни пукнатини.

Клучни зборови: испукани порозни средини, модел на еквивалентен континуум, двојно порозен модел, модел со дискретни пукнатини, споредба на моделите, гранични елементи

NUMERIČKO UPOREĐIVANJE KONCEPTUALNO RAZLIČITIH MODELA PROTOKA I TRANSPORTA U POROZNOJ SREDINI

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Rezime

Značaj istraživanja procesa tečenja i transporta efluenata u poroznim sredinama podstakao je razvoj čitavog niza različitih numeričkih modela koji služe za prognozu tih fenomena. U ovom članku je izvršeno upoređivanje tri različita modela za izučavanje tečenja podzemnih voda i transport zagađujućih efluenata: model ekvivalentnog kontinuuma (EC), model dvojne poroznosti (DP) i nehomogeni model (NM) sa diskretnim pukotinama. Mada je jasno da se ta tri modela baziraju na sasvim različitim

predpostavkama u pogledu njihove validnosti, u dostupnoj literaturi do sada nije vršeno uporedno istraživanje u kakvim okolnostima dva od njih ili sva tri – daju slične rezultate. Autori su koristili metodu graničnih elemenata sa dvojnim reciprocitetom, šemu sa multidomenom, i podrobno objasnili njenu implementaciju pri rešavanju ovog složenog zadatka. Takva numerička šema je prvi put korišćena u modelima sa dvojnom poroznošću. Pokazala je zadovoljavajuću tačnost i veliku fleksibilnost u pripremama modela, posebno u slučaju nehomogenih mreža sa diskretnim pukotinama.

Ključne reči: porozne sredine sa pukotinama; model ekvivalentnog kontinuuma; dvojno porozni model; model sa diskretnim pukotinama; upoređivanje modela; granični elementi