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Modelling of processes in fractured rock using FEM/FVM on multidimensional domains ☆

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Abstract

The paper deals with a new approach to the numerical modelling of groundwater flow in compact rock massifs.

Empirical knowledge of hydrogeologists is summarized first. There are three types of objects important for the groundwater flow in such massifs—small fractures, which can be replaced by blocks of porous media, large deterministic fractures and lines of intersection of the large fractures. We solve problem of the linear Darcy's flow on each of these three separated domains and then we join them by coupling the equations. We do not require geometrical correspondence between 1D, 2D and 3D meshes, which simplifies the process of the spatial dicretization. The mixed-hybrid FEM with the lowest-order Raviart–Thomas elements is used for approximation of the solution. The advective mass transfer is solved by the FVM on the same discretization as the flow problem.

Results of numerical experiments with the model are shown in the end of the paper.

Keywords: Fractured rock; Groundwater flow; Finite element method; Mixed-hybrid FEM; Finite volume method; Multidimensional domain

1. Introduction and motivation

Our research is motivated by the need of finding the most suitable locality for a permanent deep repository of radioactive waste in the Czech Republic. The process of selection and some preliminary projects already began. The models presented here are outcomes of one of these projects. Described numerical models are intended to be used for simulations of the flow and transport processes in the large neighborhood of the repository (socalled far-field), which was a task exceeding the possibilities of existing models.

2. Principal ideas of fluid flow model in fractured rock environment

The radioactive waste repository will be situated in a compact crystalline rock massif. The hydrogeological research has brought following empirical knowledge about the rock environment and groundwater flow in them:

- The rock matrix can be considered hydraulically impermeable.
- Even the most compact massifs are disrupted by numerous fractures.

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- Most of these fractures are relatively small ones, with the characteristic length less than one meter.
- The groundwater flow in the small fractures is extremely slow.
- Small fractures have significant total volume and play an important role in the transport processes.
- Most of the liquid is conducted by a relatively small number of large fractures. Their characteristics are usually known.
- The fastest flux of groundwater is observed on intersections of large fractures. These lines behave like a "pipelines" in the massif.

These facts lead us to the conclusion that there are three different types of objects involved in the conduction of groundwater through the compact rock: small fractures, large fractures and intersections of the large fractures.

The previous works in the field of numerical modelling of processes in fractured rock proved, that small fractures could be replaced by equivalent porous media by using the techniques of homogenization, described for example in [2,3]. The large fractures and their intersections could not be homogenized, the discrete fracture network approach must be used—see [1,2]. This approach is unsuitable for the small fractures due to its computational costs.

As a result of the previous paragraphs, we can say that the model of groundwater flow and contaminant transport in the compact rock massifs should incorporate 3D porous blocks, 2D fractures and 1D lines. We have three different domains in the area of interest, which are hydraulically connected. This problem is similar to the double-porosity approach used in the models of transport in porous media [4]. However, the double-porosity models use domains of the same dimension, with no potential flow in one of the domains and with the mass-exchange between the domains driven by diffusive processes. These three facts constitute a difference between our problem and the problem of transport in the double-porosity environment.

3. Approximation of the flow problem in each domain

We will show an approximation of the flow problem in each of the three domains without communication with the other ones.

We have three domains Ω_i, i is an index denoting the dimension $i \in \{1, 2, 3\}$. Ω_1 is a set of line segments placed in 3D space, Ω_2 is a set of polygons placed in 3D space and Ω_3 is a set of simply connected three-dimensional domains. We can define a potential driven flow on Ω_1, Ω_2 and Ω_3. The governing equations are the linear Darcy's law and the continuity equation:

$$\mathbf{u}_i = -\mathbf{K}_i \cdot \nabla p_i \quad \text{on } \Omega_i, \tag{1}$$

$$\nabla \cdot \mathbf{u}_i = q_i \quad \text{on } \Omega_i, \tag{2}$$

where $\mathbf{u}_i$ is the velocity of the flow ($\mathbf{u}_2$ has to lie in the particular polygon, $\mathbf{u}_1$ has to have the direction of the particular line), p_i is the pressure (piezometric) head, $\mathbf{K}_i$ is the second-order tensor of hydraulic conductivity ($i \times i$ symmetric, positive definite matrix) and q_i is the function expressing the density of sources/sinks of the fluid. We prescribe three types of boundary conditions on $\partial\Omega_i$—the Dirichlet, the Neumann and the Newton:

$$p_i = p_{iD} \quad \text{on } \partial\Omega_{iD}, \tag{3}$$

$$\mathbf{u}_i \cdot \mathbf{n}_i = u_{iN} \quad \text{on } \partial\Omega_{iN}, \tag{4}$$

$$\mathbf{u}_i \cdot \mathbf{n}_i - \sigma(p_i - p_{iD}) = u_{iN} \quad \text{on } \partial\Omega_{iW}, \tag{5}$$

where p_{iD}, u_{iN} and σ are given functions.

For the approximation of these three problems we use the mixed-hybrid FEM with the lowest-order Raviart–Thomas elements on tetrahedras in Ω_3, triangles in Ω_2 and line segments in Ω_1. More rigorous formulation of the continuous problem and the derivation of the discretized problem can be found in [6,5] for the problem in Ω_3, in [7] for the problem in Ω_2 and in [8] for the problem in Ω_1.

The discretization leads to the system of linear equations:

$$\mathbb{S}_i \mathbf{x}_i = \mathbf{r}_i, \tag{6}$$

where $\mathbf{x}_i = [\mathbf{u}_i, \mathbf{p}_i, \boldsymbol{\lambda}_i]^{\mathrm{T}}$, $\mathbf{r}_i = [\mathbf{r}_{i1}, \mathbf{r}_{i2}, \mathbf{r}_{i3}]^{\mathrm{T}}$ and

$$\mathbb{S}_i = \begin{pmatrix} \mathbb{A}_i & \mathbb{B}_i & \mathbb{C}_i \\ \mathbb{B}_i^{\mathrm{T}} & & \\ \mathbb{C}_i^{\mathrm{T}} & & \mathbb{F}_i \end{pmatrix}.$$

The $\boldsymbol{\lambda}_i$ are traces of the pressure head on the sides of the mesh.

4. Connection of the independent problems

Now we will show how to connect the three independent problems presented in previous section and how to express the mass exchange between the domains Ω_1, Ω_2 and Ω_3. We can do that on the level of the discretized problem due to properties of the mixed-hybrid formulation.

First, we join the three systems (6) into one large system

$$\mathbb{S}\mathbf{x} = \mathbf{r}, \tag{7}$$

where $\mathbf{x} = [\mathbf{x}_3, \mathbf{x}_2, \mathbf{x}_1]^{\mathrm{T}}$, $\mathbf{r} = [\mathbf{r}_3, \mathbf{r}_2, \mathbf{r}_1]^{\mathrm{T}}$ and

$$\mathbb{S} = \begin{pmatrix} \mathbb{S}_3 & & \\ & \mathbb{S}_2 & \\ & & \mathbb{S}_1 \end{pmatrix}.$$

4.1. Conforming and non-conforming connection of the elements

We allow two different kinds of connections of the elements with different dimensions, called *conforming* and *non-conforming*. This fact makes our model unique from the most of other numerical models using the elements of different dimensions. These models (such as FEFLOW) allow only conforming connections.

The difference between these connections is shown in Fig. 1.

The conforming connection requires the element of lower dimension placed exactly on a side or an edge of the element of higher dimension. This connection seems to be a natural way of connecting the elements in the FEM models, but it leads to very complicated algorithms for the mesh generation, when the solved problem has complex geometry of the domain (such as fractured rock massifs).

This is the reason for allowing the other kind of the elements' connections—socalled non-conforming. In this case, there is no requirement on the spatial position of the communicating elements, the only requirement is on their sizes. We should use approximately the same discretization parameter h_i in places where the meshes intersect.

4.2. Mass exchange in the conforming connection between two elements

We will start the derivation of the equations for the mass exchange for the simple case—conforming connection between two elements. The derivation will be shown on the case of 1D and 2D elements, the case of the connection of 2D and 3D elements is completely analogous.[1]

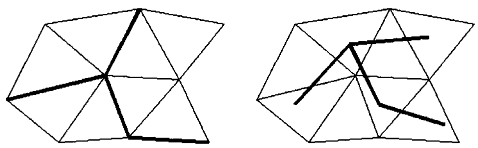

Fig. 1. Example of the conforming and non-conforming connection of the elements.

[1] We do not allow direct conforming connection of 1D and 3D elements, because there is no direct way how to express flux through an edge of a 3D element in our 3D model.

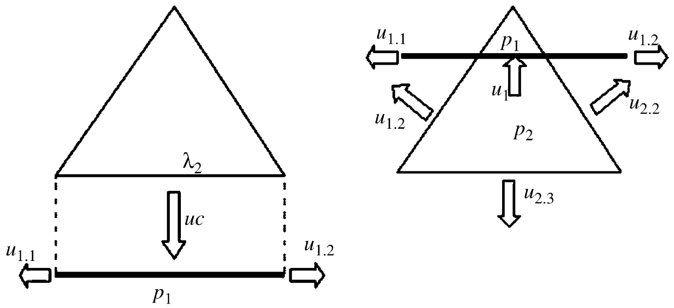

Fig. 2. Fluxes and pressure heads for the conforming (left) and non-conforming (right) connections of 1D and 2D elements. (The elements in the left picture are drawn separated and shifted in the direction of the dotted line.)

The situation is drawn in Fig. 2.

First let us examine the original state. The marked side of the triangular element is considered as an external side of the 2D mesh. We assume the homogenous Neumann boundary condition on this side:

$$u_C = 0. \tag{8}$$

This equation can be found as one line of the block $\mathbb{C}_2^{\mathrm{T}}$ of the matrix $\mathbb{S}_2$ and right-hand side $\mathbf{r}_{23}$. For the 1D element, there is a mass balance equation written in the form:

$$-u_{1,1} - u_{1,2} = 0, \tag{9}$$

which can be found in block $\mathbb{B}_1^{\mathrm{T}}$ of the matrix $\mathbb{S}_1$ and the vector $\mathbf{r}_{12}$.

Now we express the exchange of the mass between the elements. We consider that the flux u_C between 2D and 1D elements is proportional to the pressure heads gradient between the elements

$$u_C = \sigma_C(\lambda_2 - p_1), \tag{10}$$

λ_2 is the pressure head on the side of the 2D element, p_1 is the pressure head in the center of the 1D element and σ_C is the coefficient of proportionality. The mass balance equation for the 1D element can be written as

$$u_C - u_{1,1} - u_{1,2} = 0. \tag{11}$$

We can rewrite Eqs. (10) and (11) as

$$u_C - \sigma_C\lambda_2 + \sigma_C p_1 = 0, \tag{12}$$

$$\sigma_C\lambda_2 - u_{1,1} - u_{1,2} - \sigma_C p_1 = 0. \tag{13}$$

If we compare (8) with (12) and (9) with (13), we notice, that it is sufficient to add or subtract coefficient σ_C to four elements of the matrix and we make the desired connection between the system $\mathbb{S}_1\mathbf{x}_1 = \mathbf{r}_1$ and $\mathbb{S}_2\mathbf{x}_2 = \mathbf{r}_2$. The changes in the matrix $\mathbb{S}$ are shown in Fig. 3.

This procedure has to be repeated for each pair of elements connected by the conforming connection.

4.3. Mass exchange in the case of non-conforming connection of the elements

As in the previous section, we will show the derivation on the example of 1D and 2D elements, the procedure is the same for the other two cases (1D with 3D and 2D with 3D). The situation is shown in Fig. 2. The flux u_I between elements is proportional to the pressure head gradient. We can express it like

$$u_I = \sigma_I(p_2 - p_1), \tag{14}$$

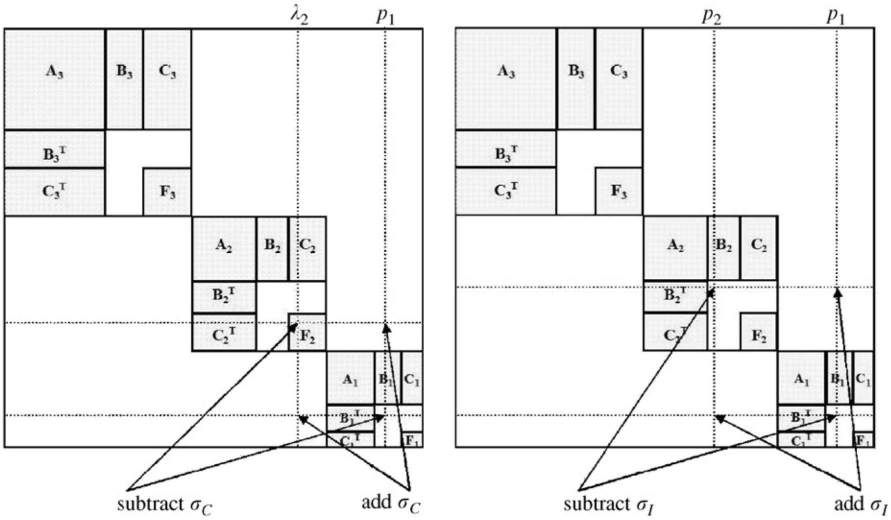

Fig. 3. Setting up a conforming (left) and non-conforming (right) connection between 1D and 2D elements in the matrix $\mathbb{S}$.

where p_2 is the pressure head in the center of the triangular element and p_1 is the pressure head in the center of the linear element. The coefficient σ_I has to reflect the size of the intersection of the elements and the distance of their centers. We write the mass balance equation for the triangular element:

$$-u_{2,1} - u_{2,2} - u_{2,3} - u_I = 0, \tag{15}$$

where $u_{2,1}$, $u_{2,2}$, $u_{2,3}$ are fluxes through the sides of the triangle. For the linear element, the mass balance equation is

$$-u_{1,1} - u_{1,2} + u_I = 0, \tag{16}$$

where $u_{1,1}$, $u_{1,2}$ are fluxes through the ends of the linear element. If we substitute (14) to (15) and (16) we obtain:

$$-u_{2,1} - u_{2,2} - u_{2,3} - \sigma_I p_2 + \sigma_I p_1 = 0, \tag{17}$$

$$-u_{1,1} - u_{1,2} + \sigma_I p_2 - \sigma_I p_1 = 0. \tag{18}$$

It can be seen that the non-conforming connection can be realized by adding, resp. subtracting the value σ_I to elements of the matrix $\mathbb{S}_C$ shown in Fig. 3.

This procedure has to be repeated for each pair of the elements connected by the non-conforming connection.

5. Modelling of the transport phenomena

Our model simulates a basic convective transport process described by an equation of the form:

$$\partial_t C + \nabla \cdot (C\mathbf{u}) = q_m \quad \text{on } \Omega, \tag{19}$$

where C is an unknown concentration of the solution and q_m is a source term. We use the finite volume method for approximation of this equation. We can perform this calculation on the same mesh as we have used for the calculation of the flow field, due to the direct calculation of the inter-element fluxes in the mixed-hybrid FEM. An existence of elements with various spatial dimension causes no need for any modification of the standard FVM scheme. Therefore, we can use standard tools for solving the above stated equation.

However, Eq. (19) is only the most simple description of the transport processes in underground. A numerical model based on this equation could be used for problems, where there is a relatively fast flux of groundwater, only one dissolved contaminant and the interaction between contaminant and the solid phase can be neglected. Unfortunately, the simulation of the radioactive waste repository does not meet any of these assumptions. For such simulation we have to have generally n contaminants in our model. The contaminants interact mutually in the solution and with the surrounding rock environment. The radioactive decay of the contaminants is also significant in this case. Finally, the velocity of the flow is very low therefore the diffusion–dispersion processes are significant. The equation describing the transport processes for this kind of problem is

$$\partial_t \beta(C_i) - \nabla \cdot (\mathbf{D}\nabla C_i) + \nabla \cdot (C_i \mathbf{u}) + R_i(C_1, \ldots, C_n) = q_{mi} \quad \text{on } \Omega. \tag{20}$$

Here C_i is the concentration of the ith contaminant, $\beta(\cdot)$ represents time evolution and equilibrium adsorption reaction, $\mathbf{D}$ is diffusion–dispersion tensor, $R_i(\cdot)$ represents changes of concentration of the ith contaminant due to chemical and radioactive reactions and q_{mi} is a source term for the ith contaminant.

A numerical model of this equation on the multidimensional domain will use the operator splitting technique and will be introduced in a forthcoming paper.

6. Implementation and example of results

We have implemented this approach for solving the flow problem and the transport phenomena in the programming language C. Results of benchmark problems show that the hydraulic communication and the mass exchange between

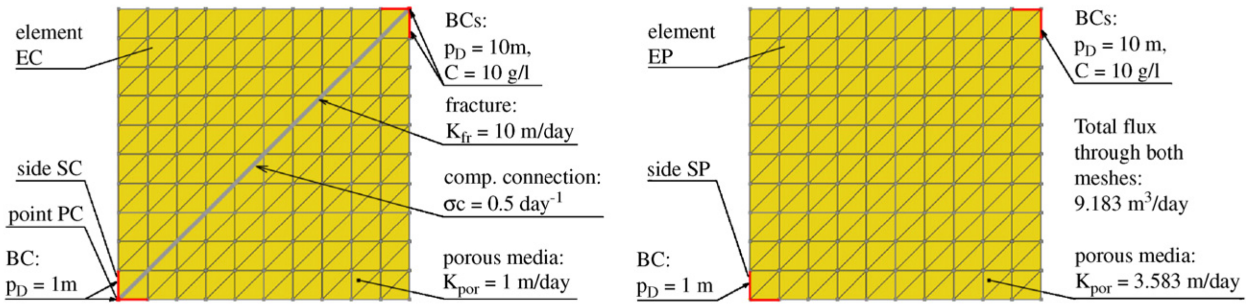

Fig. 4. Domains, meshes, parameters and observation points for the transport problems.

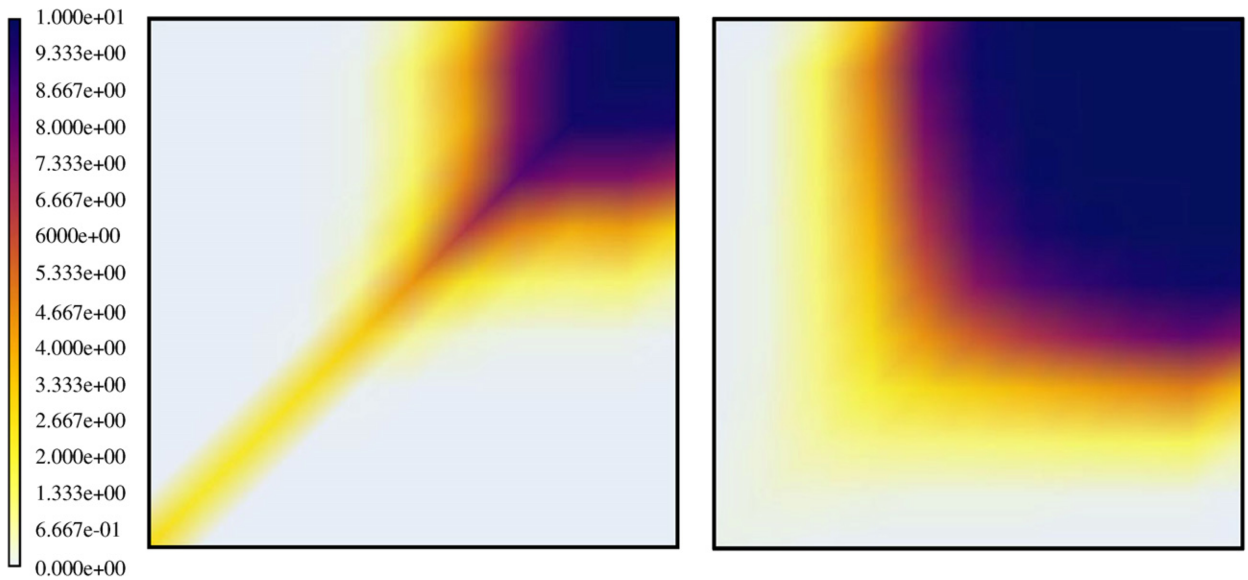

Fig. 5. Concentration field at time 4 days for the domain with fracture (left) and equivalent porous media domain (right).

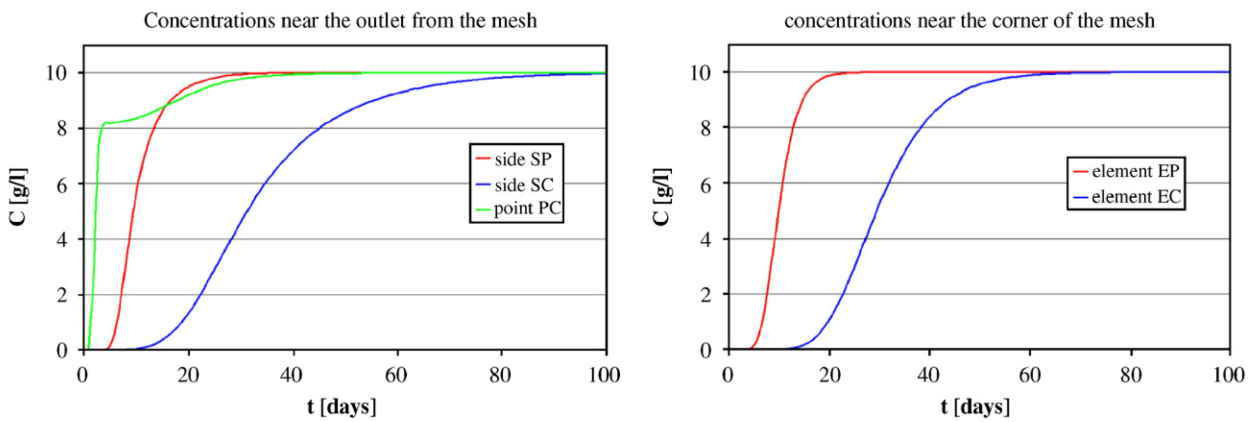

Fig. 6. Evolution of the concentrations in the selected points of the mesh.

elements of various dimensions works well and the behavior of the groundwater calculated by our program has properties of behavior of the groundwater in real fractured rock massifs.

In order to demonstrate the difference between the equivalent porous media approach and our new approach, let us consider the following benchmark problem, whose settings are shown in the left part of Fig. 4.

We took a square shaped domain, with a diagonal fracture inside. On such domain we calculated the flow problem, with predictable result, most of the fluid went through the fracture.

Next, we have tried the equivalent porous media approach for the same problem. We used the same domain, with the same boundary conditions, but without the fracture. We used an approach for the setting up a global permeability of the REV (reference elementary volume) of a fractured rock. We calibrated the value of the permeability K_{por}—constant in whole domain—of the porous media to obtain the same flux through the domain as in the previous case, as shown in right part of Fig. 4. The results of the following calculation clearly proved, that the shape of the flow field in this problem is totally different from the previous problem.

Even more significant difference can be observed in the results of the advective transport model, which are shown in Figs. 5 and 6. We have to emphasize again the fact that the transport model we used for this calculation is very simple. Therefore its results must be considered as a visualization of the flow field, not as a realistic simulation of the mass transfer process.

7. Conclusion

We have introduced a way how to set up a numerical model of groundwater flow and transport in fractured rock environment. Our approach uses the mixed-hybrid FEM on three hydraulically connected domains and FVM for the transport.

There are some open problems and unanswered questions concerning this approach:

- Although the results of the tests seem to be quite positive, we still know nothing about behavior of our model in large, real-world hydrogeological problems.
- We have to define an algorithm for prescribing the values of the coefficients σ_C and σ_I. This algorithm will be based on our experiences gained by calculation of the real-world problems. These two coefficients will be good parameters for the calibration of the models.
- Still there is no rigorous theoretical background for the new model. We have proved the existence and uniqueness of the solution and estimated the error for all three models we used for the construction of the new one. Proofs for the new model are goals for the theoretical works in a forthcoming paper.

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