A new approach for the numerical modelling of the groundwater flow in the fractured rock massifs

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Abstract A new approach to the modelling of the groundwater flow in fractured rock is presented in the paper. The empirical knowledge of the hydrogeologists is summarized first. There are three types of objects important for the groundwater flow—small fractures, which can be replaced by blocks of porous media, large deterministic fractures and lines of intersection of the large fractures. These objects are by their nature 3-D, 2-D and 1-D, respectively. The rest of the paper describes how to set up a numerical model representing all three types of objects. We use existing models based on the Mixed-Hybrid FEM and we connect them by equations representing the mass exchange between various types of elements. Our model uses two types of connection of the elements, the so-called *compatible* and *incompatible* types.

Key words FEM; fractured rock; groundwater flow; numerical modelling

INTRODUCTION AND MOTIVATION

Numerical modelling of the hydraulic, geochemical and transport processes in fractured rock has attracted the attention of many scientists for more than 40 years. The first numerical models of such processes were created in the late 1960s of the 20th century. According to Diodato (1994), more than 30 software packages existed that claimed to solve the problem of fluid flow in fractured rock in 1994.

Despite these facts, there are a lot of open and unresolved problems in this field of research. The reason for such situation lies in the nature of the problem. Lack of input data, their uncertainty and often low accuracy, high computational costs are the main difficulties we encounter when we try to simulate processes in fractured rock. Avoiding these difficulties is usually possible only at a price of simplification of the problem.

Our research is motivated by the need to find the most suitable locality for a permanent deep repository of radioactive waste. There are two nuclear power plants in the Czech Republic, a construction of the repository is planned in the 2030s of the 21st century. The process of selection of the most suitable locality has already begun, as well as some other preliminary projects. Two of them are projects GAČR 102/04/P019 and MŽP VaV 660/2/03, focused on improving and testing existing numerical models and development of the new models. In this paper, we will show one of the results of these projects, a new approach for numerical models of groundwater flow which could be used for simulations of the processes in the large neighbourhood of the repository.

PRINCIPAL IDEAS OF THE MODEL OF FLUID FLOW IN FRACTURED ROCK ENVIRONMENT

The radioactive waste repository will be situated in the compact crystalline rock massif. Of course, a good and reliable numerical model of the fluid flow and transport in such a massif has to reflect its specific properties. The hydrogeological research brought the following empirical knowledge about the rock environment there and the groundwater flow in them:

(a) The rock matrix can be considered hydraulically impermeable.
(b) Even the most compact massifs are disrupted by numerous fractures.
(c) Most of these fractures are relatively small ones, with the characteristic length less than 1 m.
(d) The groundwater flow in the small fractures is extremely slow.
(e) On the other hand, these small fractures have significant storativity capacity and play an important role in the transport processes.
(f) It is barely possible to obtain exact data for all the small fractures. They must only be treated in a statistical way.
(g) Most of the liquid is conducted by a relatively small number of large fractures. The spatial position of these fractures is usually known or detectable by field measurements.
(h) The fastest flux of groundwater is observed on intersections of large fractures. These lines of the intersection behave like "pipelines" in the compact rock massifs.

These facts lead us to conclude that there are three different types of objects involved in the conduction of groundwater through compact rock: small fractures, large fractures and intersections of the large fractures. Now let us examine these objects from the point of view of numerical modelling.

The small fractures

As previously stated, in most cases there is a large number of small fractures in the massif. However, we usually know only the data of statistical kind (such as distribution of poles) about the fractures. There are two possible approaches to the modelling of the flow in such environment: *the stochastic discrete fracture networks* or *the homogenization and replacement with porous media*.

The first one is more suitable for small problems (spatial dimension of the domain up to tens of metres) but for the large problems (such as simulations of the massif with the repository) we encounter serious problems (mainly of the computational nature) with usage of that approach (Cacas *et al*., 1990).

On the other hand, the second approach is much more applicable for large problems. Fractured rock disrupted only by small fractures can be relatively well homogenized and replaced by a porous media with equivalent hydraulic properties. The methods of the homogenization and setting the hydraulic parameters of the replacing porous media can be found for example in Kirkpatrick (1971), Bear (1993) or Bogdanov (2003).

The large fractures

The situation here is almost opposite to the previous one. The large fractures are relatively well known and not numerous, but causing strong heterogeneity of the environment. The methods of homogenization lead to serious errors and inaccuracies in this case. However, *the discrete fracture networks* approach (not stochastic) works well, even for large problems if we consider only the large fractures.

The DFN approach usually represents the fractures as two-dimensional (2-D) objects (circular discs, polygons, etc.) placed in the 3-D space. The transversal dimension of the fractures is at least 100 times smaller than the other two dimensions, so the representation as 2-D objects causes no significant loss of accuracy of the model. The transversal dimension of the fracture effects the values of permeability tensor as shown in Bear (1993) or Adler & Thovert (1999).

The intersections of the large fractures

This case is similar to the previous one. The objects of this type are relatively rare in the rock massif, but significant for the fluid flow. The velocity of the flow on the intersection of fractures can be higher in order of magnitude than the velocity in the fractures. Fortunately, the velocity is still low enough for holding the assumption of the potential flow governed by Darcy's law. For the same reasons as in the previous case we can treat the intersections as 1-D objects placed in 3-D space.

As a result of the previous paragraphs, we can say that the model of groundwater flow in the compact rock massifs should incorporate 3-D porous blocks, 2-D fractures and 1-D lines. So 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 (Chen, 1989). 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 make a difference between our problem and the problem of transport in the double-porosity environment.

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 in this section.

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

$$u_i = -K_i \cdot \nabla pi \quad \text{on} \quad \Omega_i \tag{1}$$

$$\nabla \cdot u_i = q_i \quad \text{on} \quad \Omega_i \tag{2}$$

where u_i is the velocity of the flow (u_2 has to lie in the particular polygon, u_1 has to have the direction of the particular line), p_i is the hydraulic pressure, 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 the boundary conditions on the $\partial\Omega_i$—Dirichlet's, Neumann's and Newton's:

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

$$u_i \cdot n_i = u_{iN} \quad \text{on} \quad \partial\Omega_{iN} \tag{4}$$

$$u_i \cdot n_i - \sigma(p_i - p_{iD}) = u_{iN} \quad \text{on} \quad \partial\Omega_{iW} \tag{5}$$

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. The rigorous formulation of the continuous problem and the derivation of the discretized problem can be found in Maryška *et al.* (2000) or Kaaschieter & Huijben (1992) for the problem in Ω_3, in Maryška *et al.* (2005) for the problem in Ω_2 and in Tauchman (2003) for the problem in Ω_1.

The discretization leads to the system of linear equations in form:

$$\begin{aligned} \mathrm{A}_i\, \mathrm{u}_i + \quad \mathrm{B}_i\, \mathrm{p}_i + \quad \mathrm{C}_i\, \lambda_i &= r_{i1} \\ \mathrm{B}_i^T\, \mathrm{u}_i &= r_{i2} \\ \mathrm{C}_i^T\, \mathrm{u}_i + \mathrm{F}_i\, \lambda_i &= r_{i3} \end{aligned} \tag{6}$$

where λ_i are traces of the pressure on the sides of the mesh. We rewrite this system of equations in abbreviated form:

$$S_i x_i = r_i \tag{7}$$

where $x_i = [u_i, p_i, \lambda_i]$, $r_i = [r_{i1}, r_{i2}, r_{i3}]^T$ and

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

Connection of the independent problems

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

First, we join the three systems in (7) into one large system:

$$Sx = r \tag{8}$$

where $x = [x_3, x_2, x_1]^T$, $r = [r_3, r_2, r_1]^T$ and:

$$S = \begin{pmatrix} S_3 & & \\ & S_2 & \\ & & S_1 \end{pmatrix}$$

Compatible and incompatible connection of the elements

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

The difference between this two kinds of connection is shown in Fig. 1. The compatible connection requires the element of lower dimension placed exactly on the side or 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 causes serious and almost unsolvable problems at the stage of the mesh generation for problems with complex geometry of the domain. Unfortunately, the fractured rock massifs fall into this category of problems.

This is the reason for allowing the other kind of the elements' connections—so called incompatible. In this case, there is no requirement on the spatial position of the communicating elements with different dimensions, the only requirement is on their sizes. We should use approximately the same discretization parameter h_i for all three meshes to avoid the situations shown in Fig. 2.

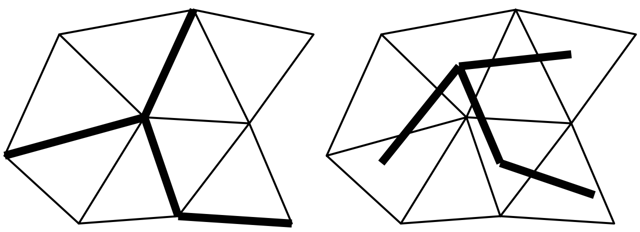

Fig. 1 Example of the compatible and incompatible connection of the elements.

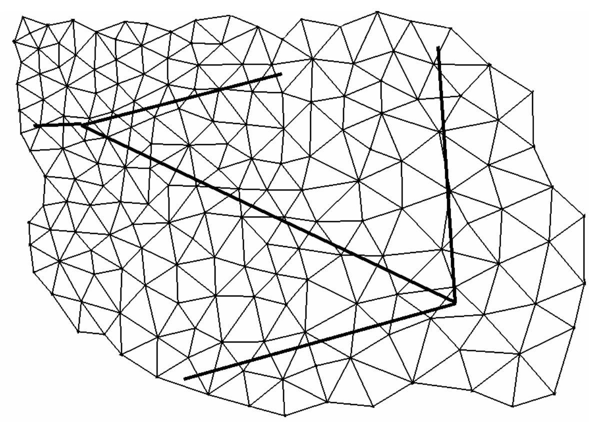

Fig. 2 An unsuitable connection of the 1-D and 2-D elements, $h_1 >> h_2$.

The mass exchange in the compatible connection between two elements

We will start the derivation of the equations for the mass exchange for the most simple case—compatible connection between two elements. The derivation will be shown in the case of 1-D and 2-D elements, the case of the connection of 2-D and 3-D elements is completely analogous. The situation is drawn in Fig. 3. We do not consider direct compatible connection of 1-D and 3-D elements. If we need to incorporate the connection of this kind to our problem, we can do this indirectly by 2-D element, connecting both these elements, or by setting the connection as incompatible.

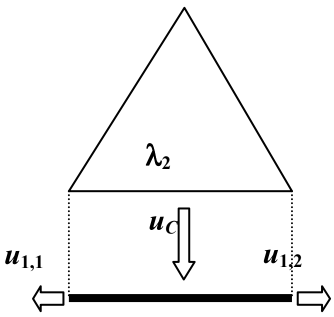

Fig. 3 Fluxes and pressures for the compatible connection of 1-D and 2-D element. (The elements are drawn separated and shifted in the direction of the dotted line.)

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

$$u_C = 0 \tag{9}$$

This equation can be found as one line of the block C_2^T of the matrix S_2 and right hand side r_{23}. For the 1-D element, there is a mass balance equation written in the form:

$$-u_{1,1} - u_{1,2} = 0 \tag{10}$$

which can be found in block B_1^T of the matrix S_1 and the vector r_{12}.

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

$$u_C = \sigma_C(\lambda_2 - p_1) \tag{11}$$

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

$$u_C - u_{1,1} - u_{1,2} = 0 \tag{12}$$

We can rewrite equations (11) and (12) as:

$$u_C - \sigma_C\lambda_2 + \sigma_C p_1 = 0 \tag{13}$$

$$\sigma_C\lambda_2 - u_{1,1} - u_{1,2} - \sigma_C p_1 = 0 \tag{14}$$

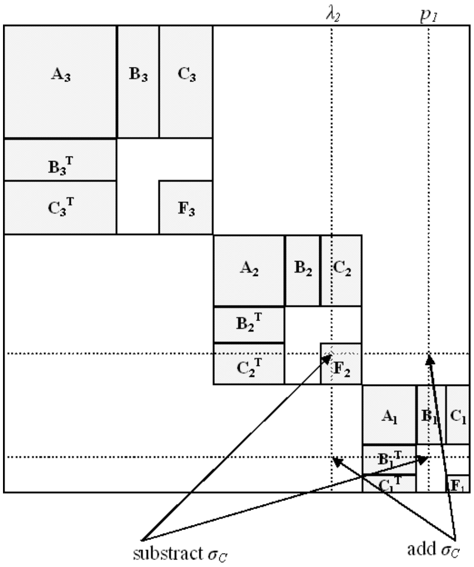

Fig. 4 Setting up a compatible connection between 1-D and 2-D element in the matrix S.

If we compare (9) with (13), and (10) with (14), 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 $S_1x_1 = r_1$ and $S_2x_2 = r_2$. The changes in the matrix S are shown in Fig. 4.

After adding values for all compatible connections (of both kinds, 1-D with 2-D and 2-D with 3-D elements) to the system (8), the matrix S changes its structure to this form:

$$S_C = \begin{pmatrix} A_3 & B_3 & C_3 & & & & & & \\ B_3^T & & & & & & & & \\ C_3^T & & F_{C3} & & E_3^T & & & & \\ & & & A_2 & B_2 & C_2 & & & \\ & & E_3 & B_2^T & D_2 & & & & \\ & & & C_2^T & & F_{C2} & & E_2^T & \\ & & & & & & A_1 & B_1 & C_1 \\ & & & & & E_2 & B_1^T & D_1 & \\ & & & & & & C_1^T & & F_{C1} \end{pmatrix} \tag{15}$$

(where F_{Ci} are modified blocks F_i and E_i are blocks created by the connecting of the elements.

The mass exchange in the case of the incompatible connection of the elements

In this section we will derive the equations describing the mass exchange between the elements of different dimensions connected incompatibly. As in the previous section,

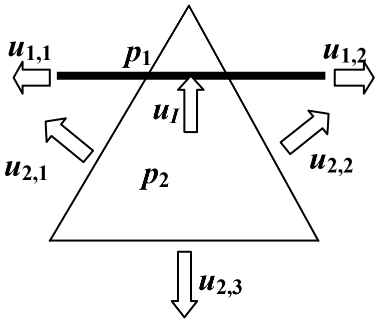

Fig. 5 Fluxes and pressures for the incompatible connection of 1-D and 2-D element.

we will show the derivation on the example of 1-D and 2-D elements, the procedure is the same for the other two cases (1-D with 3-D and 2-D with 3-D). The situation is shown in the Fig. 5.

The flux u_I between the elements is proportional to the pressure gradient as in previous case of the connection. We can express it like:

$$u_I = \sigma_I (p_2 - p_1) \tag{16}$$

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

$$-u_{2,1} - u_{2,2} - u_{2,3} - u_I = 0 \tag{17}$$

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:

$$-u_{1,1} - u_{1,2} + u_I = 0 \tag{18}$$

where $u_{1,1}$, $u_{1,2}$ are fluxes through the ends of the linear element. If we substitute (16) in to (17) and to (18) we obtain:

$$-u_{2,1} - u_{2,2} - u_{2,3} - \sigma_I p_2 + \sigma_I p_1 = 0 \tag{19}$$

$$-u_{1,1} - u_{1,2} + \sigma_I p_2 - \sigma_I p_1 = 0 \tag{20}$$

as the original mass balance equations were:

$$-u_{2,1} - u_{2,2} - u_{2,3} = 0$$

$$-u_{1,1} - u_{1,2} = 0$$

It can be seen that the incompatible connection of the elements can be realized by adding/subtracting the value σ_I to elements of the matrix S_C shown in Fig. 6.

This procedure can be repeated for each pair of the elements connected by the incompatible connection. The changes happen in the blocks D_i of the matrix (15), we call the changed block D_{Ii} and there are new blocs G_{ij}.

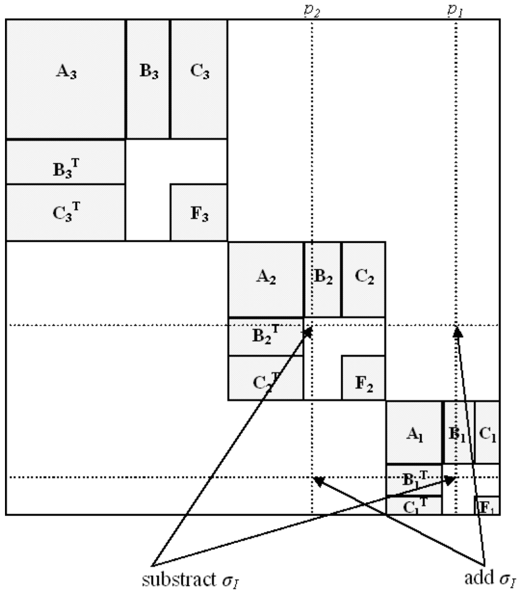

Fig. 6 Setting up an incompatible connection between 1-D and 2-D element in the matrix S_C.

Some remarks concerning the connection of the particular models

Rearrangement of the resulting matrix The matrices produced by the MH-FEM models have some special properties. The most important of them is the positive definiteness of block A. The specialized solvers of linear equations use this property of the matrix to make the process of solving more effective. Therefore it is wise to keep this property in our new model too. This goal is easy to achieve by a rearrangement of the state matrix, vector of solution, and the vector of unknowns:

$$S_{CI}=\begin{pmatrix} A_3 & & & B_3 & & & C_3 & & \\ & A_2 & & & B_2 & & & C_2 & \\ & & A_1 & & & B_1 & & & C_1 \\ B_3^T & & & D_{I3} & G_{32} & G_{31} & & & \\ & B_2^T & & G_{32}^T & D_{I2} & G_{21} & E_2 & & \\ & & B_1^T & G_{31}^T & G_{21}^T & D_{I1} & & E_1 & \\ C_3^T & & & & E_2^T & & F_{C3} & & \\ & C_2^T & & & & E_1^T & & F_{C2} & \\ & & C_1^T & & & & & & F_{C1} \end{pmatrix} \tag{21}$$

As the right-hand side we use the vector:

$$r_{CI}=[r_{31},r_{21},r_{11},r_{32},r_{22},r_{12},r_{33},r_{23},r_{13}]^T$$

the vector of unknowns has form

$$x_{CI}=[u_3,u_2,u_1,p_3,p_2,p_1,\lambda_3,\lambda_2,\lambda_1]^T$$

The domain Ω In previous text we have considered the domain Ω as:

$$\Omega=\Omega_1\cup\Omega_2\cup\Omega_3$$

providing that at least two of the three sets $\Omega_1 \cap \Omega_2$, $\Omega_1 \cap \Omega_3$, $\Omega_2 \cap \Omega_3$ are non-empty. This was a natural presumption for the purposes of the derivation of the model. If we have a model constructed by the above described procedure, we can weaken the requirement on **Ω**: It is sufficient to presume the **Ω** to be a simply connected set in the Euclidean space E_3:

$$\Omega = \Gamma_1 \cup \Gamma_2 \cup \Gamma_3 \tag{22}$$

where Γ_1 is a set of line segments placed in the three-dimensional space, Γ_2 is a set of polygons placed in the three-dimensional space, Γ_3 is a set of 3-D domains.

The boundary conditions The original requirement on boundary condition was the existence of the three non-empty parts of the boundary $\partial\Omega_{iD}$. We can weaken this requirement by the same way as we did for the domain **Ω**. Now it is sufficient to require only the existence of a non-empty part of the boundary $\partial\Omega_D$ of **Ω**, with the prescribed boundary condition of the Dirichlet's type.

EXAMPLES OF RESULTS CALCULATED BY THE MODEL

We have implemented this approach for solving the flow problem in the programming language C. The resulting program is the subject of testing at the time of writing of this paper. The first results of the testing shows that the hydraulic communication and the mass exchange between elements of various dimensions works well and the behaviour of the groundwater calculated by our program has properties of the behaviour of the groundwater in real fractured rock massifs.

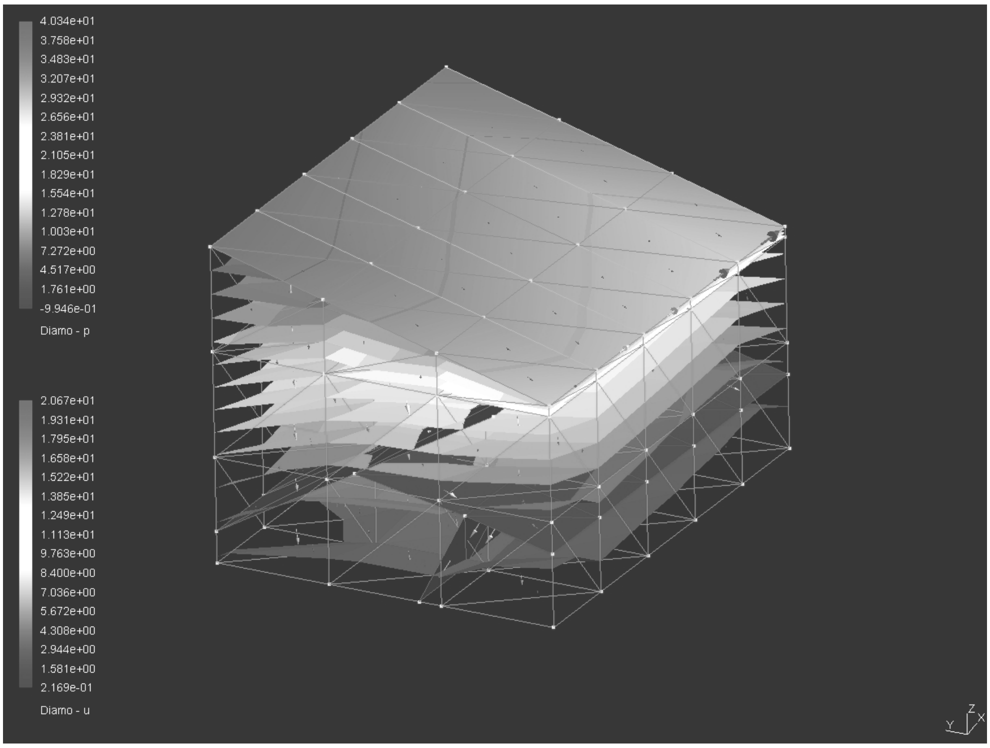

Fig. 7 Example of the results of the benchmark testing problem.

An example of one of the benchmark problems for the model of the fluid flow is shown in Fig. 7.

This problem simulates a block of sloped landscape—simulated as a porous media, disrupted by three large fractures. The triangular elements of the fractures are connected in an incompatible way with the tetrahedral elements of the porous media. There is also a set of triangular elements on the upper side of the model, for the simulation of the surface flow. The connection between these elements and porous media is the compatible one. The lowest edge of the upper side represents a water stream. There are several 1-D elements, connected compatibly with the surface elements. We have prescribed constant nonzero density of the liquid sources on the surface to simulate the rainfall. The results show that the simulated flow field is in good agreement with our expectations.

CONCLUSIONS

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

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 behaviour 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 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, uniqueness of the solution and the estimation of the error for all three models we used for the construction of the new one. These proofs for the new model are the goals of theoretical works in the next months.

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