MODELLING ADVECTIVE AND DIFFUSIVE PROCESSES IN FRACTURED POROUS MEDIA WITH FINITE ELEMENTS

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Abstract. *A conceptual model for risk assessment in an underground repository is introduced. For the numerical simulation of the problem in question governing equations are presented. A fracture-matrix model, which describes the rock masses by coupling discrete fractures and porous blocks, is used for simulation of flow and transport in a randomly generated fracture system. The governing equations are approximated by means of finite elements. For the numerical solution of the advective-diffusive equation the symmetrical streamline stabilization (S^3) is applied in order to stabilize the high advective transport in the fractures. It combines the Galerkin method with the Least-Squares method leading to oscillation-free results due to an inherent upwind effect. The procedure is used to simulate a hypothetical contamination leakage from an underground repository. The concentration distribution obtained with this model demonstrates the importance of considering the fractures in a discrete manner. For comparison results of a simulation without fractures are also presented.*

Keywords: *contamination, advection-diffusion, finite element*

1. INTRODUCTION

Viewing the increasing amount on waste production in developed countries, alternative repository concepts are being considered. In this context exploited coal mines may be used to store waste material (Jäger et al., 1990). A prerequisite for a safe waste repository is the proof that no contaminant solutes, transported through the groundwater, may reach the biosphere. In the case of sedimentary layers, like carboniferous rock or sandstone, the country rock mass in which the waste disposal is embedded is fractured and porous. Through fractures and fissures groundwater may flow with much higher velocities than in the porous matrix. Depending on the interconnectivity of the fractures, relative fast pathways may be present between the waste repository and the biosphere. In such case dilution, chemical reactions and sorption may still ensure save long-term waste disposal.

Simulation models allow a prediction of the local and temporal development of the pollutants concentration. In this paper, a model containing the fractures in the rock mass in a discrete manner is used. The rock itself is modeled as a porous medium. In this model, the essential transport processes occur in the fractures by advection. Retardation effects of the transport are attributed to the diffusion/dispersion and sorption in the porous rock. A problem one has to deal with is the numerical coupling of the fast advective transport in the fractures with the slow diffusive process in the matrix. The solution of the advection-diffusion equation by the traditional Galerkin approach becomes inefficient. In order to avoid spurious oscillations, a fine discretization is needed, leading to a huge effort concerning storage and computation time. For the numerical solution of the advective-diffusive equation the symmetrical streamline stabilization (S3) is applied in order to stabilize the high advective transport in the fractures. It combines the Galerkin method with the Least-Squares method leading to oscillation-free results due to an inherent upwind effect (Wendland and Schmid, 2000).

1.1 Waste deposition

The technical process to bring waste from the surface to the underground repository is schematized in Fig. 1. At the surface, the waste that is to be deposed is mixed with mining residues and water to obtain a fluent mass. This mass is transported by pipelines down to the level of the underground repository and finally posed there through injection tubes.

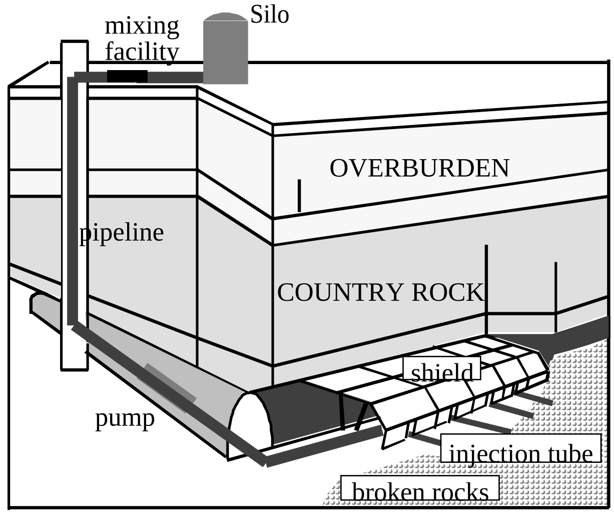

Figure 1 - Schematic representation of waste deposition in the worked coal layer.

The volume available for disposal originates from the mining process itself. The coal layer in the mine is worked out mechanically and transported to the surface leaving holes. A previously installed safety shield supports the load of the overlaying layers. After a certain time of exploitation, the shield is moved forward and the rock mass above the worked coal layer breaks into the generated hollow space, as shown in Fig. 2. The break of the rock overlaying the repository can create new fractures there or the existing fractures can open, altering the hydraulic behavior in these sediments. The layers underlying the repository do not experience such effects and can be considered undisturbed. The broken rock consists of blocks of different dimensions. Approximately 20% of this highly heterogeneous sub-region are voids. Through the injection tubes these openings are now filled with the waste mixture transforming itself into a compact solid like concrete. The area filled out by the mixture represents - for low pollutant waste - the underground repository. When the mine is exhausted, the pumps, which have kept the coal mine dry, are switched off. The groundwater level will rise and flood the repository. Its reliability will depend on the groundwater flow situation in the complex porous and fractured media in which the repository is embedded.

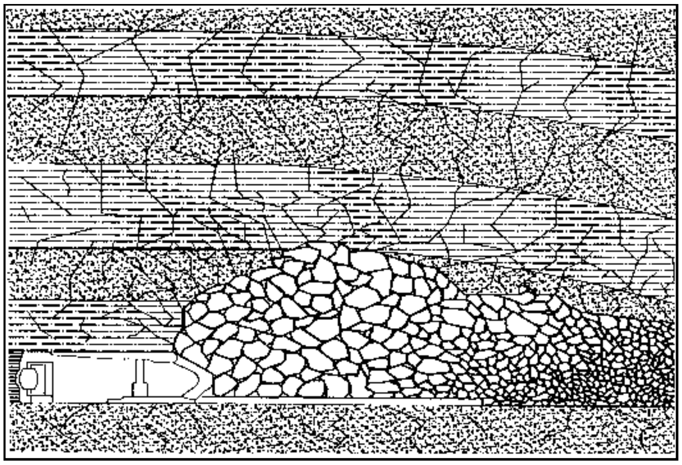

Figure 2 - Broken rocks due to mining work.

2. GOVERNING EQUATIONS

We consider a single-phase (water) flow with a single dissolved solute moving through a homogeneous, saturated porous medium. The flow field is independent of the solute concentration and is at steady state. Chemical reactions and decay will not be considered, though they can easily be incorporated into the mathematical and numerical models.

2.1 Groundwater flow

A coupled model including porous and fracture flow is chosen to simulate the hydraulic situation. We will consider the problem of steady flow of an incompressible fluid in a saturated medium. The mass balance equation in this case is given as:

$$\nabla \boldsymbol{q} = Q \tag{1}$$

where $\boldsymbol{q}$ is the specific discharge and Q represents the source terms (Bear, 1979). Assuming a piecewise isotropic and homogeneous porous medium, the specific discharge can be given by the Darcy equation, which assumes a linear relation between discharge and driving force $\boldsymbol{I}$,

$$\boldsymbol{q} = k \frac{\rho g}{\mu} \boldsymbol{I} \tag{2}$$

in which k is the permeability, ρ is the fluid density, g is the gravity acceleration and μ is the dynamic viscosity. $\boldsymbol{I}$ is defined as the negative gradient of the hydraulic potential:

$$\boldsymbol{I} = -\nabla h \tag{3}$$

For a porous medium the permeability k is a parameter determined through percolation experiments. Assuming a fracture to be defined by parallel plates, the pressure as constant across the opening and neglecting friction, the permeability k for the fracture can be approximated by (Berkowitz et al., 1988)

$$k = \frac{a^2}{12} \tag{4}$$

in which a is the opening of the fracture.

A point to be observed is that the derived governing equation differs from the classical hydrodynamic equations in that the influence of inertia or acceleration forces is not considered. Although Darcy´s Law (Eq. 2) is empirical, DeWiest (1965) showed heuristically that it is equivalent to the classic Navier-Stokes equations, when inertial terms are neglected. This fundamental difference is however, to be expected observing that due to the very large surface exposed to a fluid in a porous medium the viscous resistance will greatly exceed any inertial forces in the fluid unless turbulence sets in. Under such conditions it would be justified even a priori to neglect the inertia terms, as is indeed frequently done in treatments of the classical equations for cases in which the dominating forces are those due to the viscous resistance (Muskat, 1982). Of course, Darcy´s Law is valid as long as the assumptions chosen for the derivation are valid. At low Reynolds numbers (*i.e.*, at low velocity for a constant grain size d and viscosity) we have a region where the flow is laminar, viscous forces are predominant and the linear relationship is valid, as verified experimentally by many investigators (see, for example, Bear, 1972). The upper limit of this range for porous media is at a value of Re between 1 and 10. Indeed, considering a porous media with grain size in the order of 1-10 mm and a natural hydraulic gradient of 0.001, the Reynolds number will lye in the scale of 10^{-2} to 10^{-3}, even for a very high permeability of 10^{-10} m^2. These values confirm the validity of Darcy´s Law for the most practical cases.

2.2 Solute transport

The transient transport of dissolved solutes is governed by the advection-dispersion equation

$$\frac{\partial c}{\partial t} + \frac{\boldsymbol{q}}{n}\nabla c - \nabla(\boldsymbol{D}\nabla c) = Q\left(c^* - c\right) \tag{5}$$

where c is the solute concentration, t is the time variable, $\boldsymbol{q}$ is the specific discharge, $\boldsymbol{D}$ is the hydrodynamic dispersion tensor, containing the mechanical dispersion and molecular diffusion, c^* is the solute concentration of the sources and n is the constant effective porosity in the blocks. For the fractures n is set equal to 1.

2.3 Numerical approach

The continuity law couples the equations describing flow and transport in the fractures and in the matrix. A 3D-model combines 2-D elements for the fracture and 3-D elements for the porous matrix. Channeling effects can be considered through 1-D elements (Fig. 3).

The flow Eq. (1) will be solved using a standard approach based on the finite element method (FEM). Wendland and Schmid (1995) give a detailed discussion of this problem.

Solute transport in fractured porous media combines the high advection in fractures with the slow diffusion processes in the matrix. Due to a fine discretization in order to avoid high Peclet and Courant numbers in the fractures and to unsymmetrical system of equations resulting from the FEM approximation of Eq. (5), the use of traditional approaches leads to a great computational effort.

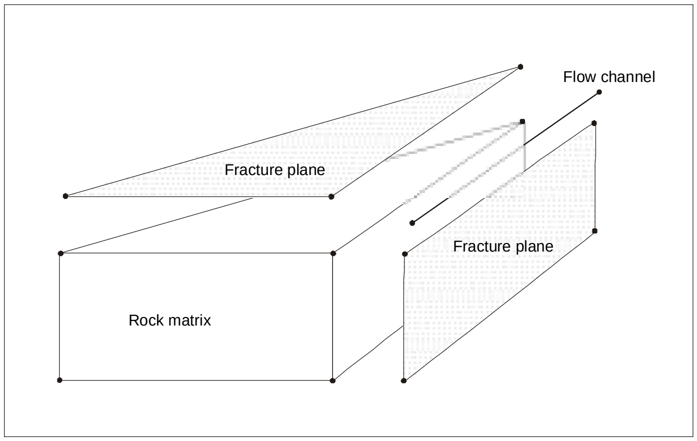

Figure 3 - Combination of different element types in a 3D-model.

We use a different formulation based on the finite element method for advection dominated transport (Wendland and Schmid, 2000). The basis of the technique is to treat the transport Eq. (5) in two steps. In the first step the dispersion part is approximated by a standard Galerkin scheme, while in the second step the advection part is approximated by the least squares method. The two parts are assembled analytically, resulting in one system of equations:

$$\left[\frac{\boldsymbol{M}}{\Delta t}+\theta\left(\boldsymbol{B}+\boldsymbol{V}\right)+\theta\boldsymbol{V}^{T}+\boldsymbol{U}^{*}\right]\boldsymbol{c}^{+} = \left[\frac{\boldsymbol{M}}{\Delta t}-\left(1-\theta\right)\left(\boldsymbol{B}+\boldsymbol{V}\right)+\theta\boldsymbol{V}^{T}-\frac{\left(1-\theta\right)}{\theta}\boldsymbol{U}^{*}\right]\boldsymbol{c}^{+}+\boldsymbol{P} \tag{6}$$

with

$$\boldsymbol{M}=\int_{\Omega}\varphi^{T}\varphi\; d\Omega$$

$$\boldsymbol{B}=\int_{\Omega}\boldsymbol{D}\nabla\varphi^{T}\nabla\varphi\; d\Omega \;+\; \int_{\Omega}Q\,\varphi^{T}\varphi\; d\Omega$$

$$\boldsymbol{V}=\frac{1}{n}\int_{\Omega}\boldsymbol{q}\varphi^{T}\nabla\varphi\; d\Omega$$

$$\boldsymbol{U}^{*}=\frac{\theta^{2}\nabla t}{n}\int_{\Omega}\boldsymbol{q}^{T}\boldsymbol{q}\;\nabla\varphi^{T}\nabla\varphi\; d\Omega$$

$$\boldsymbol{P}=\int_{\Omega}Qc^{*}\varphi^{T}d\Omega$$

Here is Δt the time step, c^{+} is the solute concentration at the new time level ($t+\Delta t$), c^{-} is the solute concentration at the old time level (t), θ is the weighting factor varying between 0 and 1 and φ is the interpolation function for the approximated solution.

The stiffness matrix results to be symmetric. Only half part of the sparse matrix has to be stored. Fast iterative algorithms for symmetric systems of equations like a preconditioned conjugate gradient method can successfully be used. The method leads to the introduction of an artificial diffusion term (U^*). Solute transport with high Peclet and Courant numbers does not lead to oscillations due to an inherent upwind damping. The upwind effect acts only in flow direction. It has no cross diffusion. The efficiency of the new formulation in terms of accuracy and computation time has been demonstrated in comparison with the standard unsymmetrical approach for many test cases (Wendland, 1995).

3. FIELD-SCALE EXAMPLE

The simulation technique described above will be used to show the behavior of a tracer as it moves through a fractured porous medium like sandstone. The domain under consideration is a rectangular section of 46m length and 27m width (Fig. 4). For the porous matrix we assumed a constant permeability of $k = 3.10^{-16}\ m^2$ and an effective porosity of $n = 0.20$.

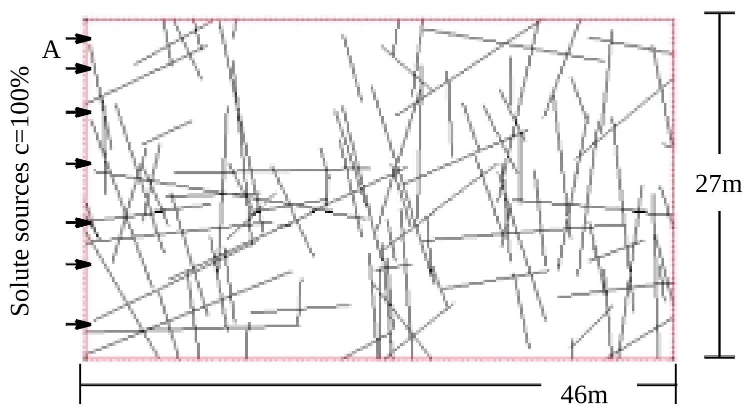

Figure 4 - Geometry of the field-scale example.

A network of one-dimensional fractures was randomly generated and distributed over the domain. The aperture of the fractures varies between $a=570\mu m$ and $a=9\mu m$ corresponding to permeability of $k = 2,7.10^{-8}\ m^2$ and $k = 6,8.10^{-12}\ m^2$ respectively. In Fig. 4 the generated fractures can be seen as straight lines.

The boundary conditions for the flow field are given by potentials of h=110m on the left and h=10m on the right side of the domain; upper and lower sides are streamlines. For the solute transport the boundary conditions consist of a specified concentration of c*=100% at seven nodes on the left side of the domain as shown in Fig. 4. The initial concentration is 0% (zero) elsewhere.

4. RESULTS AND DISCUSSION

For the simulation of the considered problem the computer code SICK100 (Schmid et al., 1991) was employed. The geometric model was discretized by 13500 nodes, dividing the rock matrix in 16900 two-dimensional elements and the fractures in 2300 one-dimensional elements. The fine discretization of the porous blocks is necessary for a correct approximation of the high concentration gradients normal to the fractures. The system of equations resulting from the finite element method was solved using a robust iterative algorithm (Schmid and Braess, 1988).

The calculated potential distributions at steady state with and without fractures are shown in Fig. 5. The different shading represents the reduction of the hydraulic potential from h=110m (left) to h=10m (right). For the case without fractures (Fig. 6a) the distribution of potentials is, as expected, parallel to the boundaries with prescribed condition. In Fig. 6b one can recognize how the fractures strongly affect the hydraulic behavior, changing the pattern of constant gradient.

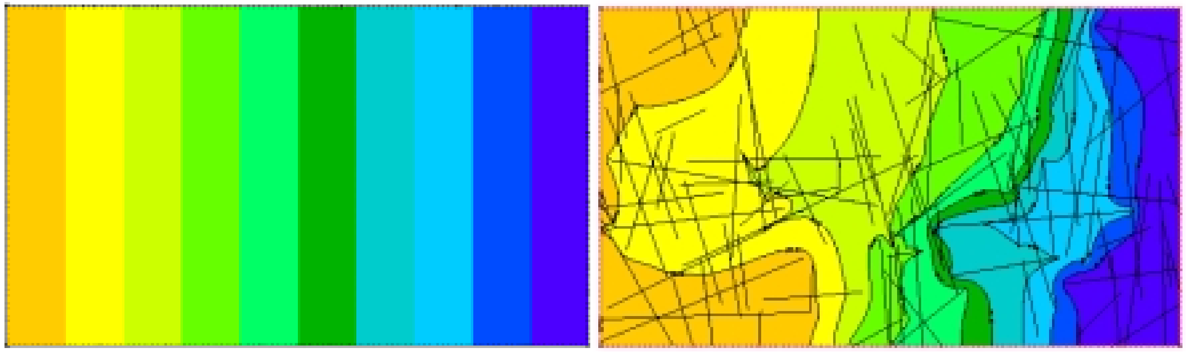

Figure 5 - Potential distribution (steady state):
a) without fractures, b) with fractures.

At a given instant (*t=0*) the concentration c*=100% at the 7 nodes at the left side was suddenly applied to the model. The transient process was simulated over a period of 2000 hours. The time step chosen had a length of 2 hours. In Fig. 6 the solute distribution after 2000 hours of simulation for the cases without (Fig. 6a) and with fractures (Fig. 6b) are shown. The different shading represents the advance of the solute front from the injection points (c=100%, gray) into the rock mass (c=0%, white) as concentration isosurfaces.

Due to the higher permeability of the fractures the groundwater moves primarily through the fracture network distributing the solutes over the domain. One can easily identify the fast pathways opened by the fractures. The solutes applied to the point A (see Fig. 4) at the left boundary do not spread strongly due to the absence of interconnected fractures with large apertures in this part of the domain. Compared with the results from Fig. 6a one can easily realize the importance of considering the fractures embedded in the porous matrix for risk analysis in case of solute transport.

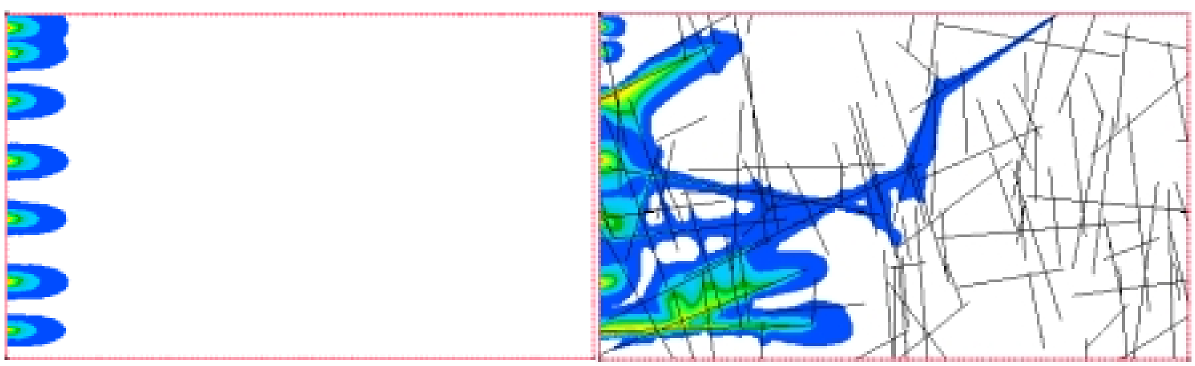

Figure 6 - Concentration distribution after 2000 hours:
a) without fractures, b) with fractures.

Although a relative fast solute spreading occurs through the fractures, it does not necessary endanger the concept of underground repositories. The concentration at the most outlying point is lower then 1%, due to the puffer effect provided by the diffusion of solute into the porous matrix as observed in Fig. 6b. This effect is strongly dependent on the diffusion coefficient, which should be determined experimentally for improved reliability of the model results.

Often such kind of simulation leads to oscillation of concentration in mesh nodes due to high Courant numbers. In order to assign this fact, breakthrough curves for some points have been investigated. Fig. 7 shows in detail a fracture cross as well as the nodes considered for the analysis. The region considered is a typical one in which mixing of contaminated with clean water can occur and oscillation can be expected. The computed breakthrough curves are shown in Fig. 8. Due to the upwind effect inherent to the S^3 scheme no oscillation is observed. Furthermore the mechanism of solute distribution through the fractures appears clearly. The solute arrives in the region contaminating first the node 1979. From this cross node the solute is distributed to adjacent nodes with different fluxes due to different fracture aperture and hydraulic gradient.

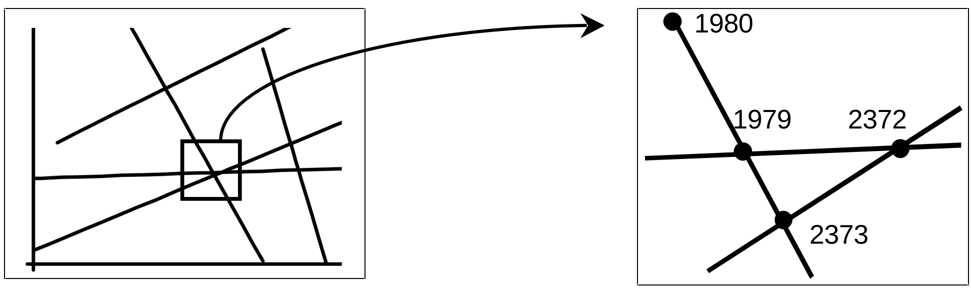

Figure 7 - Mesh detail and nodes for the breakthrough curves.

The same results were obtained using the standard (Galerkin) FEM approach. In a first evaluation, the major advantage of the S^3 scheme in comparison with the standard method appears to be the saving on computational effort. The traditional method leads to an unsymmetrical matrix, for which a direct solver was chosen. The full matrix has to be stored using a *band technique*. For the S^3 scheme a robust preconditioned conjugate gradient solver (PCG) with *sparse storage* can be used. The savings on computer memory for large models are evident. The CPU time consumed by the new method is approximately 6% of the traditional one.

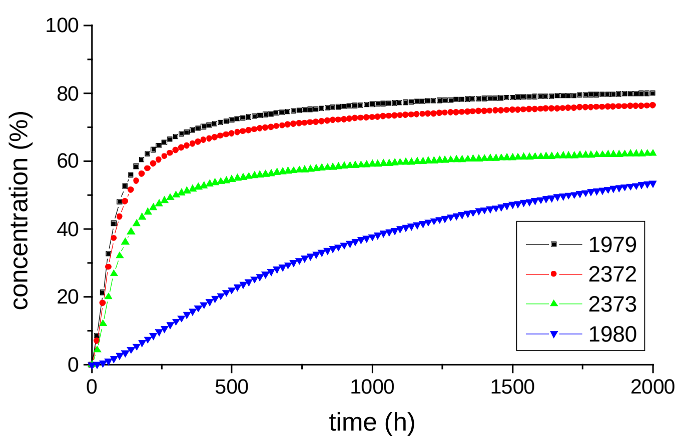

Figure 8 - Breakthrough curves for nodes depicted in Fig. 7.

5. CONCLUSION

In the context of waste disposal in an underground repository a computer simulation of groundwater flow and solute transport through a fractured porous rock has been presented for a field-scale example.

To solve the advection-dispersion equation the Symmetrical Streamline Stabilization (S^3) scheme has been applied. It provides a robust algorithm even for advection dominated problems as it occurs in the fractures. Upwind acts on the advective term assuring a stable solution without numerical oscillation, even for high advective transport. As a consequence, the computational effort in terms of time and storage could be reduced in comparison with the traditional FEM approach.

The results obtained show the importance of considering the fractures embedded in the porous rock mass in a discrete manner in order to obtain a reliable concentration distribution. Due to the higher permeability of the fractures the solutes are predominantly distributed through the fracture network over the domain. The developed method provides a useful tool for prediction of contaminant transport in risk assessment of critical facilities.

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