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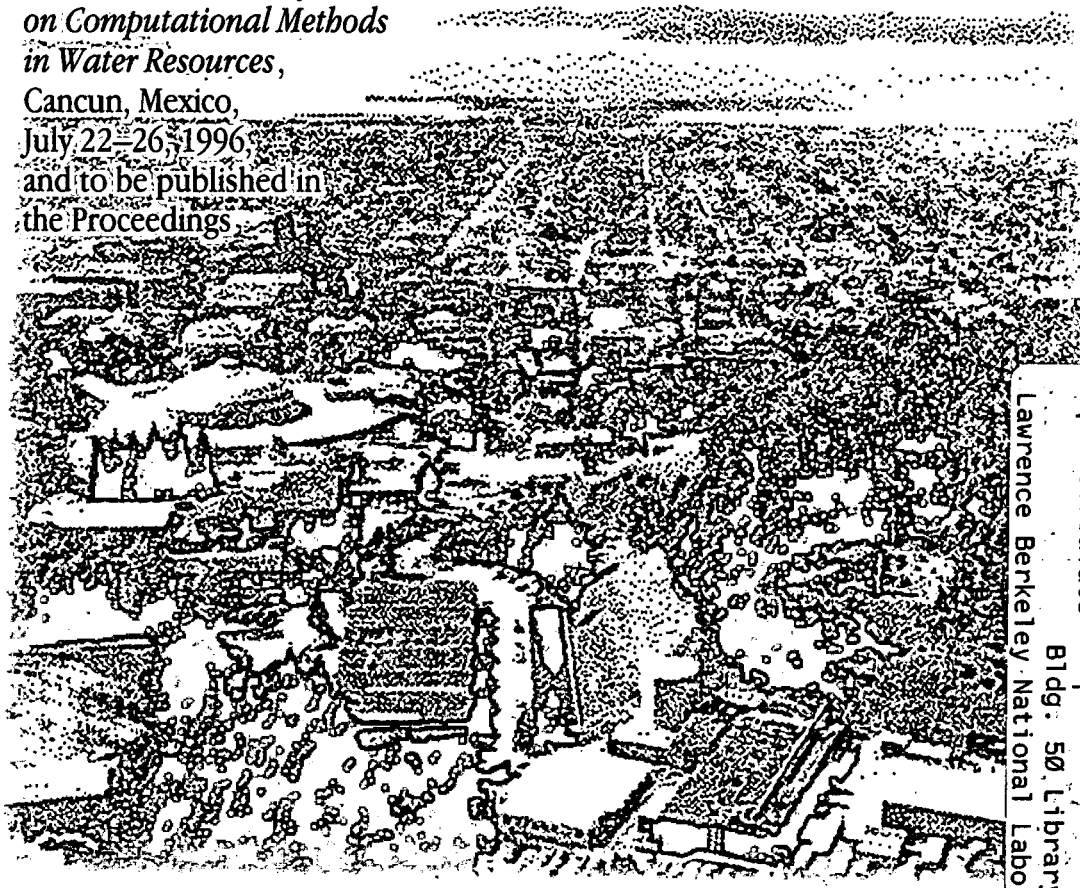

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A new Eulerian-Lagrangian finite element simulator for solute transport in discrete fracture-matrix systems

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Abstract

Fracture network simulators have extensively been used in the past for obtaining a better understanding of flow and transport processes in fractured rock. However, most of these models do not account for fluid or solute exchange between the fractures and the porous matrix, although diffusion into the matrix pores can have a major impact on the spreading of contaminants. In the present paper a new finite element code TRIPOLY is introduced which combines a powerful fracture network simulator with an efficient method to account for the diffusive interaction between the fractures and the adjacent matrix blocks.

The fracture network simulator used in TRIPOLY features a mixed Lagrangian-Eulerian solution scheme for the transport in fractures, combined with an adaptive gridding technique to account for sharp concentration fronts. Lagrangian-Eulerian schemes have been introduced in recent years to avoid numerical problems in the solution of the advection-dispersion equation. They are especially effective in advection dominated transport, which may often occur in fractures. Thus TRIPOLY is capable of handling very heterogeneous fracture networks without the need for very fine spatial or temporal discretizations.

The fracture-matrix interaction is calculated with an efficient method which has been successfully used in the past for dual-porosity models. Discrete fractures and matrix blocks are treated as two different systems, and the interaction is modeled by introducing sink/source terms in both systems. It is assumed that diffusive transport in the matrix can be approximated as a one-dimensional process, perpendicular to the adjacent fracture surfaces. A direct solution scheme is employed to solve the coupled fracture and matrix equations.

The newly developed combination of the fracture network simulator and the fracture-matrix interaction module allows for detailed studies of spreading processes in fractured porous rock. We present a sample application which demonstrate the codes ability of handling large-scale fracture-matrix systems comprising individual fractures and matrix blocks of arbitrary size and shape.

1 Introduction

In fractured reservoirs the transport of contaminants mainly occurs in a small volume of high-permeability interconnected fractures. However, most of the capacity for storing a pollutant is provided by the pore system of the rock matrix. Due to the much slower transport in the matrix, strong concentration gradients may occur from the fractures into the porous blocks. This can lead to significant solute transfer between fractures and matrix and may strongly influence the concentration field in a fractured porous formation.

Generally, the numerical simulation of flow and transport processes in fractured porous rock can be performed with either discrete models or continuum models. Discrete models describe the spatial structure of the fracture-matrix system in great detail and thus allow for a more accurate simulation than continuum models. However, the discretization and computational effort is very large, and often discrete models are limited to the fracture network only, not taking into account the rock matrix. Such discrete models, which may be called *fracture network models*, have often been used in the past, e.g. for studying dispersion phenomena or deriving equivalent continuum parameters. However, the numerical solution of advection-dispersion in fractures can become a crucial task, since natural fracture networks are very heterogeneous with regard to flow velocities, and numerical problems such as artificial dispersion or oscillations may occur.

In recent years Lagrangian-Eulerian schemes have been used more and more to avoid such numerical problems in the solution of the advection-dispersion equation (e.g [1]). The idea is to decompose the advection-dispersion equation in two parts, one controlled by pure advection and the other by dispersion. The advected concentration profiles are calculated by Lagrangian approaches such as particle tracking methods, whereas the dispersed concentration profiles are solved by conventional numerical techniques (FDM, FEM) on Eulerian grids. Karasaki [2] and Segan & Karasaki [3] introduced a Lagrangian-Eulerian finite element code TRINET for transport in two- or three-dimensional fracture networks, capable of handling heterogeneous fracture networks without numerical problems. However, like most fracture network models, TRINET does not account for solute exchange between fractures and porous rock.

In the present paper, TRINET is extended to simulate transport processes in discrete fractures embedded in porous matrix blocks. We solve the fracture-matrix interaction with an efficient numerical technique adopted from dual-porosity models (e.g. [4], [5]). Fractures and matrix blocks are treated as two different systems, and the interaction is modeled by introducing sink/source terms in both systems. We assume that the diffusive transport in the matrix can be approximated as a one-dimensional process, perpendicular to the adjacent fracture surfaces. The geometrical shape and size of the individual matrix blocks is described by polynomial functions which determine the interface area for transport in the matrix at a certain distance from the adjacent fractures. It has been shown that this method is very accurate in simulating the short-term as well as the long-term behavior in the matrix ([5]).

The fracture network simulator TRINET after Segan and Karasaki [3] and the above mentioned fracture-matrix interaction technique have been combined and incorporated in a new code TRIPOLY. It features a direct solution scheme for the coupled fracture-matrix equations to avoid iterative procedures. In the following sections we briefly describe the numerical solution and present a sample application, showing that TRIPOLY allows for detailed studies in complex fracture-matrix systems.

2 Governing Equations

In the following paragraphs, the governing equations and the numerical solution are presented only for the transport part. The flow problem is similar but less complicated and at this point we assume that it has been solved. We assume that the global transport processes take place only in the fractures; the matrix does not contribute to those processes. However, local concentration differences between the fractures and the matrix lead to a solute exchange at the interface and portions of the solute diffuse into the matrix pores.

2.1 Fractures

In the Eulerian formulation, the advection-dispersion equation for single fractures is given by

$$\frac{\partial C}{\partial t} + q\frac{\partial C}{\partial x'} - D\frac{\partial^2 C}{\partial x'^2} + \frac{W^{D1} + W^{D2}}{(2b)} = 0, \qquad (2.1)$$

where C is concentration, q is velocity, D is the dispersion coefficient, (2b) is the fracture aperture and x' is a coordinate defined along the fracture axis. W^{D1} and W^{D2} denote diffusive losses from the fracture into the adjacent matrix blocks via fracture wall one and two, respectively.

2.2 Matrix Blocks

As the transport in the matrix is much slower than the spreading in the fractures, it can be approximated as a one-dimensional process, perpendicular to the adjacent fractures. Thus we can formulate a one-dimensional diffusion equation for each matrix block in the domain (see figure 1)

$$n^M \frac{\partial C^M}{\partial t} - \frac{1}{A(s)} n^M D^M \frac{\partial}{\partial s}\left(A(s)\frac{\partial C^M}{\partial s} \right) = 0, \qquad (2.2)$$

where C^M is concentration in the matrix, n^M is porosity, D^M is molecular diffusion coefficient and s is a local coordinate perpendicular to the adjacent fractures. The latter is zero at the fracture-matrix interface. Its upper limit is s=S, which is the maximum orthogonal distance of any location inside the block to the nearest fracture. A(s) is the interface area for transport in the matrix blocks at a distance s from the surface. Hence, for s=0 this area is equal to the block surface, and, for blocks of limited extent, it steadily decreases when approaching the block center (s=S). In TRIPOLY, the interface area is defined as a polynomial of s, following a concept proposed by Pruess and Karasaki [6]. For regularly shaped blocks, interface-functions can easily be calculated from analytical expressions. For irregular blocks, a random procedure is applied.

Two boundary conditions are needed to solve the diffusion problem in eq. (2.2). First, the concentration in fractures and matrix blocks is equal at the fracture-matrix interface. This implies that the diffusion equations for individual blocks are independent from each other; the local concentration profile in the matrix is only affected by the concentration in the adjacent fractures. Second, there is a zero-flux boundary condition at s=S, i.e. in the middle of the blocks.

The diffusive solute exchange per unit fracture wall area is obtained by applying Fick's law at the interface between fractures and matrix

$$W^D = n^M D^M \left. \frac{\partial C^M}{\partial s} \right|_{s=0} . \qquad (2.5)$$

In fact, W^D in eq. (2.5) is the coupling term between eq. (2.1) of the fractures and eq. (2.2) of the individual matrix blocks, respectively.

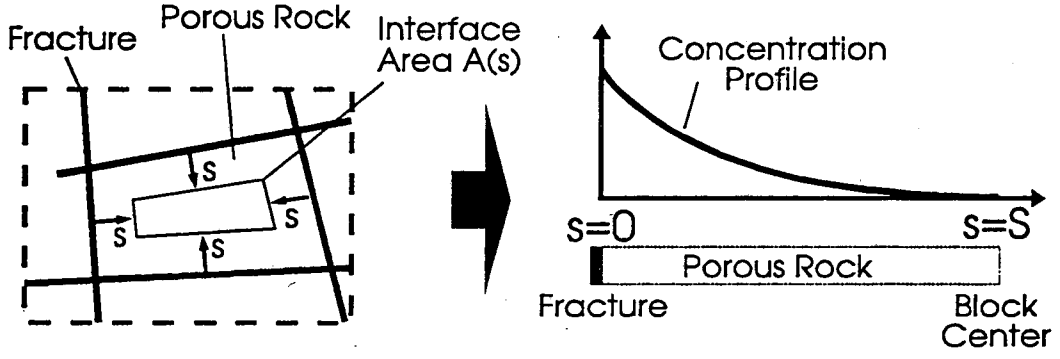

Fig. 1: One-dimensional concentration profile in matrix blocks

3 Lagrangian-Eulerian Scheme for the Fracture Network

TRIPOLY treats the advective-dispersive transport in the fracture network with a mixed Eulerian-Lagrangian finite element scheme. Prior to that, the flow field is solved with a simple Galerkin finite element method. Note that the flow field simulation is done for the fracture network only; the matrix blocks are assumed to be impermeable.

According to the Lagrangian-Eulerian method, the advection-dispersion equation (2.1) is decomposed in two parts, one controlled by pure advection, the other controlled by dispersion-diffusion. The advective concentration profile is calculated by a particle tracking technique, whereas the dispersed concentration profile is solved by a Galerkin finite element method on the Eulerian grid. Often, adaptive gridding schemes are combined with the advection part, introducing new grid nodes around sharp concentration fronts. However, numerical dispersion may occur when the advected front is projected back to the fixed Eulerian grid. Furthermore, the accuracy of the results depends on the number of particles in the model. Following the work of Segan and Karasaki [3], TRIPOLY features two major improvements compared to the above mentioned methods. First, the advective tracking in the fracture network is performed for nodal concentrations and not for particles. Therefore, the number of particles introduced in the model is not an issue. Second, numerical dispersion is avoided by creating new Eulerian grid points instead of interpolating the advected profile back to the fixed Eulerian grid.

The advective transport is performed in two steps, both using the method of characteristics. In a first step, the *Single Step Reverse Particle Tracking* method (SPRT) is applied, calculating the concentrations of fixed nodes by mapping back their characteristic. The advected concentration of any node j at time t+dt, $C(x_{j,t+dt}, t+dt)$, is equal to $C(x_{j,t}, t)$, with $x_{j,t}$ given by

$$x_{j,t} = x_{j,t+dt} - \int_t^{t+dt} q \, dt \qquad j=1,2,...J \qquad (2.8)$$

where dt is time step size , $x_{j,t+dt}$ is the location of node j at time t+dt and J is the total number of nodes. If the tracked point, $x_{j,t}$, does not correspond to a fixed node, a linear interpolation scheme is used to determine $C(x_{j,t}, t)$.

In a second step, *Continuous Forward Particle Tracking* (CFPT) is performed in the vicinity of sharp fronts. The node j is tracked forward along the streamline to the point $x_{j,t+dt}$, given by

$$x_{j,t+dt} = x_{j,t} + \int_{t}^{t+dt} q \, dt \qquad j=1,2,...J. \qquad (2.9)$$

The concentration at this point and time t+dt, $C(x_{j,t+dt}, t+dt)$, is equal to that at point j and time t, $C(x_{j,t}, t)$. If the tracked point, $x_{j,t+dt}$, does not correspond to a fixed node, a new Eulerian node is created to preserve the exact location of the front. This avoids the use of interpolation schemes when mapping back from the Lagrangian grid to the Eulerian grid, and numerical dispersion is minimized. If the sharp front has passed through the area, the created nodes are not needed anymore and can be eliminated. Thus, at every time step the element catalog has to be revised and nodal points have to be renumbered. Of course, the geometry of the fracture network itself has to preserved, and original nodes, which are located at fracture intersections, cannot be eliminated.

The new concentration profile at the end of the advection stage becomes the initial-value for the dispersion-diffusion calculation in the second stage. The equation is solved with a standard Galerkin finite element scheme using linear shape functions. As already mentioned, the simulation is performed with the new Eulerian grid which contains both fixed nodes and newly generated nodes.

Note that the solute exchange terms W^{D1} and W^{D2} are only included in the dispersion-diffusion part, not in the advective part. Thus, the advective problem is solved without taking the retarding effects of matrix diffusion into account. A correction is made in the second stage while solving the dispersion part. This procedure gives rise to some numerical dispersion for large time steps.

4 Solution Scheme for the Matrix Blocks

Each individual matrix block in the domain is associated with a one-dimensional diffusion equation, describing the local transport in the matrix. As the concentration profiles in matrix blocks do not directly affect each other, the different diffusion equations are independent. However, each of these equations is coupled to the advection-dispersion equation of the fracture network via the solute exchange terms W^{D}.

TRIPOLY features a direct solution technique for the coupled equations, originally proposed for dual-porosity models ([4], [5]). In each time step, the independent matrix diffusion equations are solved prior to the solution of the dispersion-diffusion equation of the fracture network, using a standard Galerkin finite element scheme. The fracture concentrations of the current time step are still unknown at this stage which means that the boundary condition at the fracture-matrix interface must be treated as a variable. However, it is possible to evaluate the mass transfer term (2.5) in linear dependence of the unknown fracture concentrations. Then, the mass transfer terms of all matrix blocks are inserted into equation (2.1) and a linear solver can be applied to obtain the nodal concentrations of the fracture network. Finally, the concentration profiles of the porous matrix blocks are evaluated by a backward substitution. See details in [7].

5 Coupling the Fracture Network and the Matrix Blocks

As stated in previous paragraphs, we describe the solute transport in each individual matrix block by a one-dimensional diffusion equation. However, the assumption of only *one* concentration profile being associated to each matrix block requires that all the fractures adjacent to that specific block have a constant concentration value (according to the boundary condition at the interface). Of course, this cannot be guaranteed in the numerical scheme. TRIPOLY solves this problem by assigning a number of one-dimensional concentration profiles to each block, depending on the number of finite element fracture nodes located on the fracture-matrix interface of the block. Physically, all these profiles should have the same concentration value in the center of the block. However, this requirement cannot always be met since the different diffusion equations associated to a matrix block are solved independently, and the resulting profile is mainly influenced by the concentration at the fracture-matrix interface. Our simulation results show, though, that the concentration differences at the block centers are very small, and that the effect of such differences is negligible with respect to the solute transfer between fractures and matrix blocks.

Figure 2 illustrates the concept of coupling the fracture network and the matrix blocks. Each matrix block in the model area is defined by its material properties (porosity and molecular diffusion), by geometrical parameters (interface function and block size S) and by a number of concentration profiles, corresponding to the number of adjacent fracture nodes. At the same time, each node of the fracture network is connected to a certain number of blocks, i.e. one block for dead-end-nodes, two blocks for nodes in between fracture intersections, and more than two blocks for fixed nodes located on fracture intersections. Each of those node-block connections is related to a one-dimensional concentration distribution in the matrix.

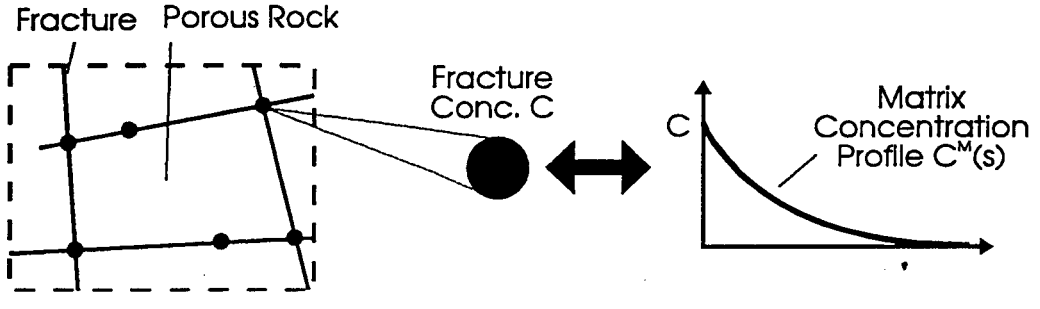

Fig. 2: Coupling fractures and matrix blocks

6 Sample Problem

The sample problem concerns advective-dispersive transport in a complex fracture network including diffusion into the porous matrix blocks. The fracture network comprises two orthogonal sets of 600 fractures each in a 10 m x 10 m square flow region. We assume that the fractures have uniform properties, i.e. uniform angles between the fractures and the x-direction, a fracture aperture of 0.8×10^{-4} m, a fracture length of 1.0 m and a longitudinal dispersivity of 0.05 m. The matrix blocks in the domain have identical hydraulic properties, with a porosity of 0.02 and a molecular diffusion coefficient of 0.2×10^{-8} m^2/s. However, the size and shape of the blocks varies significantly.

Figure 3 shows the flow domain with 5668 fractures embedded in 2337 matrix blocks. Dead-end fractures have been removed. The original finite element mesh comprises 3520 nodes. However, this number increases within the simulation due to adaptive gridding. Two noflow boundary conditions are given at the upper and lower boundaries. The left and right boundaries are associated with hydraulic heads of 0.1 m and 0.0 m, respectively. We assume that the left boundary of the model area is contaminated with a Dirichlet-type boundary condition C=1. Solutes released at this boundary are carried through the fracture network and leave at the right (outflow) boundary. Without matrix diffusion particles would cross the entire model area within less than 10^6 s. However, due to the diffusive exchange between fractures and matrix pores the transport in the fractures is strongly retarded. After 0.5×10^7 s solutes just begin to reach the outflow boundary; after 3.0×10^7 s concentrations at the outflow boundary are close to the input concentration C=1.

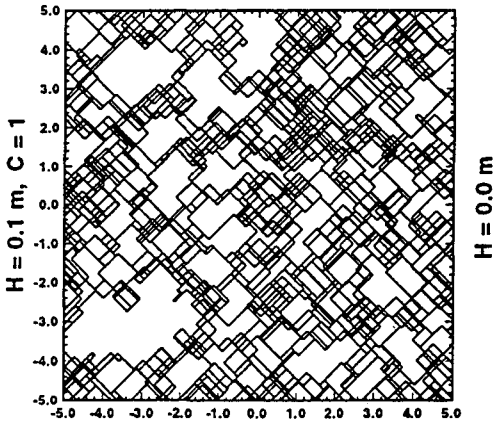

Fig. 3: Fracture network

Figure 4 shows the contaminant concentration in each matrix block at times 0.5×10^7 s and 3.0×10^7 s, respectively. For the sake of visualization, average values have been calculated out of the one-dimensional concentration profiles associated with each block.

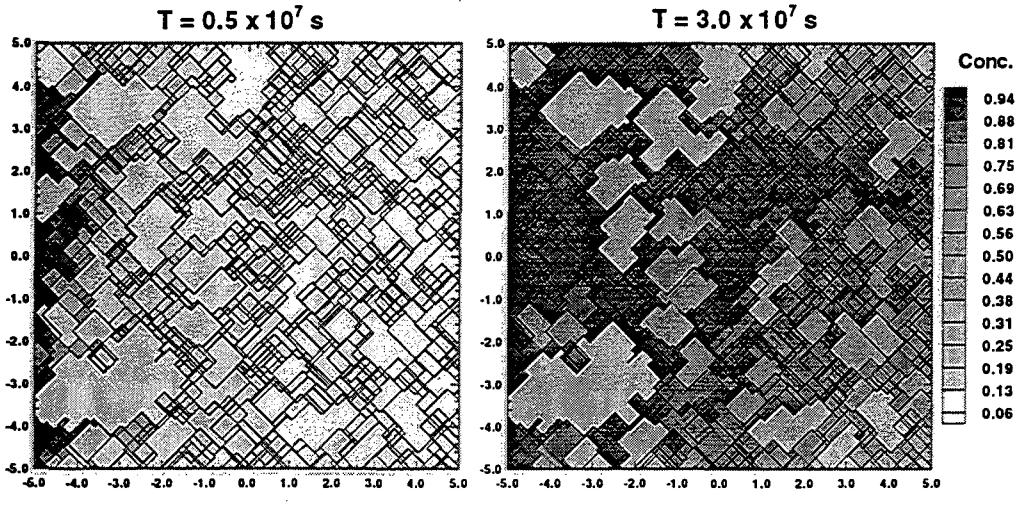

Fig. 4: Average concentration in the matrix blocks

It is apparent from Figure 4 that individual matrix blocks exhibit a very different response to the contaminant build-up in the fracture network. The concentration values vary significantly, due to the different size and shape of the blocks. Large blocks which offer a larger pore volume for storing contaminants

are much less contaminated than small blocks. As observed by Jansen et. al [8] this phenomenon can have a strong impact on the assignment of equivalent continuum parameters for the matrix blocks, a problem associated with the use dual-porosity models.

The contaminant build-up in the matrix blocks is slower than in the fractures. At 0.5×10^7 s only the blocks in the left half of the model area exhibit a build-up of contaminant concentration. Even after 3.0×10^7 s, when the fractures and most of the small matrix blocks are contaminated with concentrations close to C=1, the larger blocks in the model area are still fairly clean, with concentration values being significantly lower than in the surrounding fractures.

7 Summary and Conclusions

A finite element simulator TRIPOLY is presented for studying solute transport in discrete fracture-matrix systems. The advection-dominated flow in the fracture network is solved by a mixed Lagrangian-Eulerian scheme, while the diffusive transport in matrix blocks is modeled by a one-dimensional finite element scheme. The heterogeneous components, fractures and matrix, are treated as two different systems, coupled by a solute exchange term. However, no iterative procedures are needed, since a direct solution technique is applied. The code is capable of modeling solute transport in complex fracture-matrix systems comprising individual fractures and matrix blocks of arbitrary size and shape.

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fracture network simulator; Lagrangian-Eulerian finite element method; matrix diffusion

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