LBNL-39503
UC-000

ERNEST ORLANDO LAWRENCE BERKELEY NATIONAL LABORATORY

A New Lagrangian-Eulerian Finite Element Method for Modeling Contaminant Transport in Fractured Porous Formations

J. Birkholzer and K. Karasaki
Earth Sciences Division

September 1996
Presented at the
Second North American Rock Mechanics Symposium,
Montreal, Quebec, Canada,
June 19–21, 1996,
and to be published in
the Proceedings

REFERENCE COPY
Does Not
Circulate
Bldg. 50 Library.
Copy 1
LBNL-39503

DISCLAIMER

This document was prepared as an account of work sponsored by the United States Government. While this document is believed to contain correct information, neither the United States Government nor any agency thereof, nor the Regents of the University of California, nor any of their employees, makes any warranty, express or implied, or assumes any legal responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by its trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof, or the Regents of the University of California. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof or the Regents of the University of California.

LBNL - 39503
UC - 000

A New Lagrangian-Eulerian Finite Element Method For Modeling Contaminant Transport In Fractured Porous Formations

Jens Birkholzer and Kenzi Karasaki

in Proceedings of the 2nd North American Rock Mechanics Symposium, NARMS 96
Montreal/Quebec/Canada/19-21 June 1996

Earth Sciences Division
Ernest Orlando Lawrence Berkeley National Laboratory
University of California
Berkeley, CA 94720

September 1996

This work was supported by a NATO-Postdoctoral Scholarship, provided by the *German Academic Exchange Organization (DAAD)*, Bonn, Germany, and a Feodor-Lynen-Postdoctoral Scholarship, provided by the Humboldt-Foundation, through the U.S. Department of Energy Contract No. DE-AC03-76SF00098.

A new Lagrangian-Eulerian finite element method for modeling contaminant transport in fractured porous formations

Jens T. Birkholzer, Kenzi Karasaki
Lawrence Berkeley National Laboratory, Earth Sciences Division, Berkeley, California, USA

ABSTRACT: Fracture network simulators have been extensively 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 Lagrangian-Eulerian approach for solving flow and transport in networks of discrete fractures with an efficient method to account for the diffusive interaction between the fractures and the adjacent matrix blocks. The code is capable of handling large-scale fracture-matrix systems comprising individual fractures and matrix blocks of arbitrary size, shape, and dimension.

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, especially for advection-dominated problems (e.g. Neuman 1984). 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 (1986) introduced a Lagrangian-Eulerian finite element code TRINET for transport in two- or three-dimensional fracture networks (Segan and Karasaki, 1993). This code is capable of handling heterogeneous fracture networks without numerical problems. However, like most fracture network models, it does not account for solute exchange between fractures and porous rock. In the present paper, the code of Segan and Karasaki is extended to simulate transport processes in discrete fractures embedded in porous matrix blocks.

Several attempts have been made in the past to include fracture-matrix interaction in discrete fracture models. A straightforward technique would be to fully discretize both the fractures (planar elements in 3D-space) and the matrix blocks (volume elements in 3D-space), and simultaneously solve for solute transport in the entire domain. However, due to the strong heterogeneity of the fractured porous formation, a very fine discretization is needed in the

matrix blocks, especially at the fracture-matrix interface. Thus, simulation runs become very costly in terms of computer time and space; even for small-scale problems reasonable limits may be exceeded.

Other workers consider global flow and transport processes only for the fracture network, while using simplified approaches for the fracture-matrix interaction. A very simple model is to work with a retardation factor associated to the fractures. This approach, however, is not very exact, since it is not able to describe the time-dependence of the fracture-matrix interaction. A better representation has been achieved by simulating the local transport in the matrix with a simple analytical solution for one-dimensional diffusion into a semi-infinite half-space (e.g. Bibby 1981). This approach is good in approximating the short-term response to perturbations when steep gradients occur at the fracture-matrix boundary, but does not accurately describe the long-term behavior, since the accumulation of solute in matrix blocks of limited size cannot be modeled.

In this paper we solve the fracture-matrix interaction with an efficient numerical technique adopted from dual-porosity models (e.g. Huyakorn et al. 1983, Birkholzer 1994). Again, 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 transport in the matrix can be approximated as a one-dimensional process, perpendicular to the adjacent fracture surfaces. However, the geometrical shape and size of the individual matrix blocks is now described by so-called proximity functions which determine the fraction of matrix volume within 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 (Birkholzer, 1994).

The fracture network simulator TRINET after Segan and Karasaki (1993) 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 describe the numerical solution and present two sample applications. We shall demonstrate 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 shall be 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. The model at the present time is limited to two-dimensional fracture-matrix systems; however, the approach can be extended easily to three-dimensional problems.

We assume that the global transport processes take place only in the fracture network; the rock medium does not contribute to those processes. However, local concentration differences between the fractures and the matrix lead to a local solute exchange at the interface and portions of the solute may be stored in 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 Block*

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. 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 the concept of proximity-functions which was originally proposed by Pruess and Karasaki (1982). The proximity-function Prox(s) expresses the total fraction of matrix volume V(s) within a distance s from the adjacent fractures, divided by the total block volume V

$$\mathrm{Prox}(s) = V(s)/V\,. \tag{2.3}$$

Then, the interface area is simply the derivative of the proximity-function, multiplied with the total block volume

$$A(s) = \frac{dV(s)}{ds} = V\frac{d\,\mathrm{Prox}(s)}{ds}. \tag{2.4}$$

For regularly shaped blocks, proximity-functions can easily be calculated from analytical expressions. For irregular blocks, a random procedure is needed to derive proximity functions. A number of points are randomly distributed in each block, and the vertical distance to the nearest fracture is measured. Then, the value of the proximity-function at the coordinate s is given by the fraction of points within a distance s from the fracture surfaces, divided by the total number of points. Finally, the results of the random procedure are approximated by a best-fit-polynomial. Such a polynomial has to be determined for each matrix block in the domain.

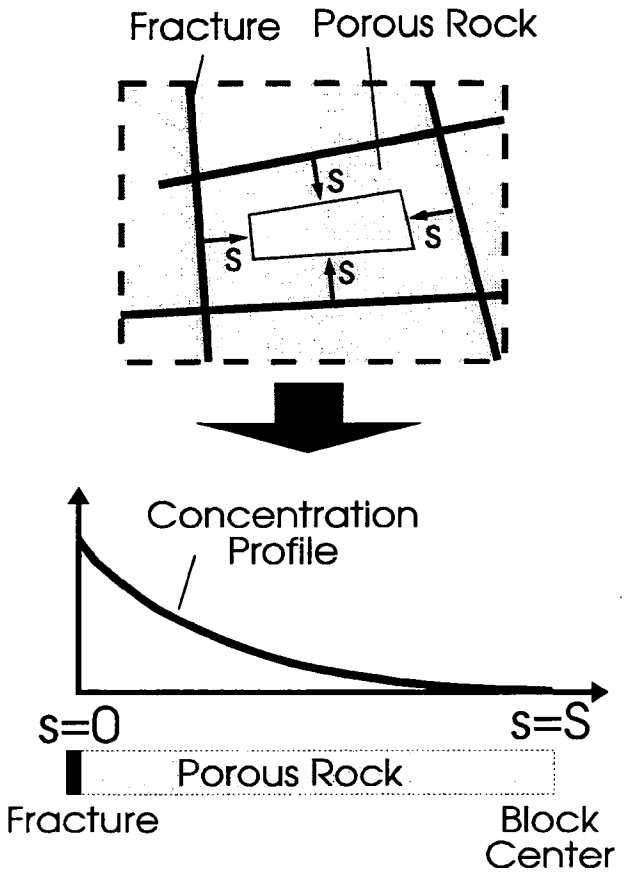

Fig. 1: One-dimensional concentration profile in matrix blocks

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

$$C^M(s=0) = C\,. \tag{2.5}$$

Second, there is a zero-flux boundary condition at s=S, i.e. in the middle of the matrix blocks

$$\frac{\partial C^M}{\partial s}(s=S) = 0. \tag{2.6}$$

These boundary conditions imply 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.

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

$$W^D = n^M D^M \left.\frac{\partial C^M}{\partial s}\right|_{s=0}. \tag{2.7}$$

In fact, W^D in eq. (2.7) is the coupling term between eq. (2.1) of the fractures and eq. (2.2) of the individual matrix blocks, respectively.

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 (1993), 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 node j at time t+dt, $C(x_{j,t+dt}, t+dt)$, is given by that of point $x_{j,t}$ which is tracked backward along the flow path

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

$$C(x_{j,t+dt}, t+dt) = C(x_{j,t}, t), \qquad (2.9)$$

where $x_{j,t+dt}$ is the location of node j, $C(x_{j,t}, t)$ is the concentration at $x_{j,t}$ and time t, dt is time step size and J is the 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 $x_{j,t+dt}$, and the concentration at this point and time t+dt, $C(x_{j,t+dt}, t+dt)$, is given by that at point j and time t

$$x_{j,t+dt} = x_{j,t} + \int_t^{t+dt} q \, dt \qquad j=1,2,...J \qquad (2.10)$$

$$C(x_{j,t+dt}, t+dt) = C(x_{j,t}, t). \qquad (2.11)$$

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 some interpolation scheme 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 located in fracture intersections cannot be eliminated.

For both backward and forward tracking, a complete mixing procedure is applied in fracture intersections. This makes the performance of TRIPOLY sensitive to the time step length. During large time steps, particles are advected along various fracture segments. Then, extensive branching takes place, and the computation becomes very inefficient. On the other hand, if time steps are chosen too small, a large number of time steps are needed to move a concentration front throughout the model area. To avoid these problems, TRIPOLY features an adaptive time step control which optimizes the time step length with regard to the above mentioned criteria.

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 the fixed nodes and the 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 this coupled equation system, originally proposed for dual-porosity models (Huyakorn et al. 1983; Birkholzer 1994).

In each time step, the independent matrix diffusion equations are solved prior to the solution of the dispersion-diffusion equation of the fracture network. Thus, the fracture concentrations of the current time step are still unknown at this stage which means that boundary condition (2.5) must be treated as a variable. However, as shown later, it is possible to evaluate the mass transfer term (2.7) 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.

In the following paragraph, the solution procedure will be described briefly. The individual matrix diffusion equations are solved by a one-dimensional standard Galerkin finite element procedure. Since this method is widely used in groundwater hydraulics, it will not be explained in this paper. Application of the Galerkin technique to equation (2.2) finally yields a tridiagonal set of equations for each matrix block which can be represented in the following manner

$$\begin{vmatrix} b_1 & c_1 & 0 & . & . & 0 & 0 \\ a_2 & b_2 & c_2 & 0 & . & . & 0 \\ 0 & a_3 & . & . & 0 & . & . \\ . & 0 & . & . & . & 0 & . \\ . & . & 0 & . & . & c_{N-2} & 0 \\ 0 & . & . & 0 & . & b_{N-1} & c_{N-1} \\ 0 & 0 & . & . & 0 & a_N & b_N \end{vmatrix} \bullet \begin{vmatrix} C_1^M \\ C_2^M \\ . \\ C_n^M \\ . \\ C_{N-1}^M \\ C_N^M \end{vmatrix} = \begin{vmatrix} d_1 - W_j^D \\ d_2 \\ . \\ d_n \\ . \\ d_{N-1} \\ d_N \end{vmatrix}$$

C_n^M is the current value of concentration at node n of the one-dimensional solution domain, N is the number of nodes in the domain and a_n, b_n, c_n and d_n are known coefficients. Node number 1 is associated with the block surface (i.e. s=0) and boundary condition (2.5), node N is associated with the center of the block (i.e. s=S) and boundary condition (2.6). Linear shape functions are used with an implicit finite difference approximation for the time integration.

W_j^D denotes the solute exchange between the fractures and the matrix per unit interface area, associated with node j in the fracture domain. According to boundary conditions (2.5) and (2.6), an inflow/outflow of solute is only possible at node 1 of the matrix domain, i.e. at the fracture-matrix interface. Both the value of the solute exchange and the nodal concentrations are unknowns at this point.

Using the general Thomas algorithm (Thomas 1949), one can factorize the tridiagonal matrix into a product of lower and upper bidiagonal matrices and perform a forward elimination. After setting $w_N=b_N$, the following steps are performed

$$u_n = a_n / w_n, \quad \text{for} \quad n = N,2 \tag{2.12}$$

$$w_n = b_n - c_n u_{n-1}, \quad \text{for} \quad n = N-1,1 \tag{2.13}$$

$$g_N = \frac{d_N}{w_N} \tag{2.14}$$

$$g_n = \frac{d_n - c_n g_{n+1}}{w_n}, \quad \text{for} \quad n = N-1,2 \tag{2.15}$$

For n=1 and with $g_1=C_1^M$, one finally obtains the following expression for the solute exchange

$$W_j^D = d_1 - w_1 C_1^M - c_1 g_2 \tag{2.16}$$

Using boundary condition (2.5), the unknown concentration of the first matrix node in equation (2.16) can be replaced by the unknown concentration C_j of fracture node j. Apart from this concentration, all remaining coefficients in equation (2.16) are known. Inserting (2.16) into equation (2.1) and performing this procedure for all matrix blocks finally gives an equation system for the fracture domain which can be solved directly for the fracture concentrations.

Once the fracture concentrations C_j are obtained, the one-dimensional concentration distributions in the matrix blocks can be readily determined by performing a backward substitution as follows

$$C_1^M = C_j \tag{2.17}$$

$$C_n^M = g_n - b_n C_{n-1}^M, \quad \text{for} \quad n = 2,N \tag{2.18}$$

This completes the solution cycle for the present time step.

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 boundary condition (2.5)). 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 (such as porosity and molecular diffusion), by geometrical parameters (interface function and block size S) and by the fracture nodes of the surrounding fractures. 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. For each connection the solute exchange is calculated according to equation (2.7), and the resulting exchange rate is introduced into equation (2.1).

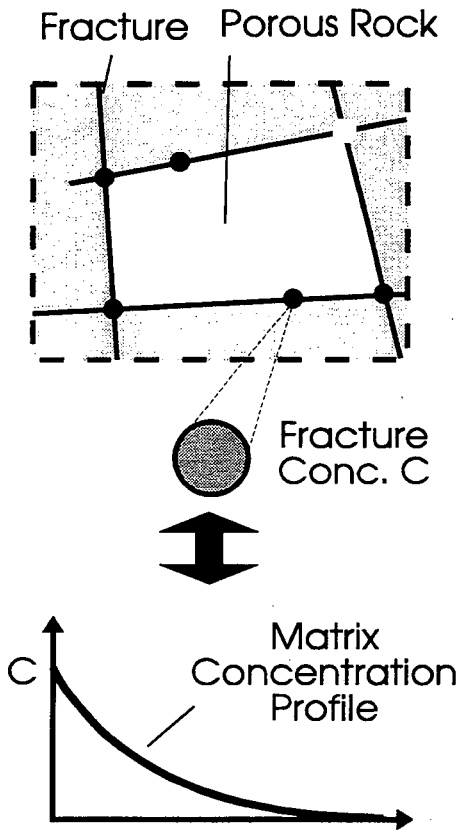

Fig. 2: Coupling fractures and matrix blocks

The adaptive gridding scheme gives rise to some problems regarding the fracture-matrix interaction. New fracture nodes, which are created during the tracking procedure, have to be connected to the adjacent blocks, and matrix concentration profiles have to be assigned to those nodes. We assume that the matrix concentration profile of a new node-matrix connection can be obtained by linear interpolation from the profiles associated to the next upstream node and the next downstream node. Extensive bookkeeping is needed to keep track of introducing and eliminating new nodes.

6 SAMPLE PROBLEMS

In this section we present two sample problems. The first problem is very simple; it is basically used to verify TRIPOLY in comparison to an analytical solution. The second problem demonstrates the codes ability to solve more complex flow and transport problems.

6.1 *Longitudinal Transport in a Single Fracture with Transverse Matrix Diffusion*

This problem concerns longitudinal transport along a single fracture and transverse diffusion into the adjacent matrix blocks. An analytical solution was developed by Tang et al. in 1981. Figure 3 schematically illustrates the problem. A contaminant source with C=1 is located in the fracture on the left boundary of the model area at x=0. The fracture aperture is 10^{-4} m. The solute is transported in the fracture due to advection and dispersion, with a flow velocity in the fracture of 0.01 m/d and a longitudinal dispersivity along the fracture axis of 0.5 m. Molecular diffusion in the fracture is chosen to 1.382×10^{-4} m^2/d. During the relatively fast transport in the fracture, part of the solute diffuses in a slow process into the adjacent porous matrix. Matrix parameters are 0.01 for the porosity and 1.382×10^{-5} m^2/d for the effective molecular diffusion coefficient. We assume that the system shown in figure 3 is part of a fractured porous formation comprising parallel fractures with a distance of 2.4 m. Thus, the matrix blocks have an infinite length and their width is 2.4 m.

For the simulation with TRIPOLY, the fracture is discretized with 10 line elements of constant length. Due to the adaptive gridding, a refined discretization adjacent to the contaminant source is not necessary. The code implicitly takes care of refining the mesh wherever it is needed.

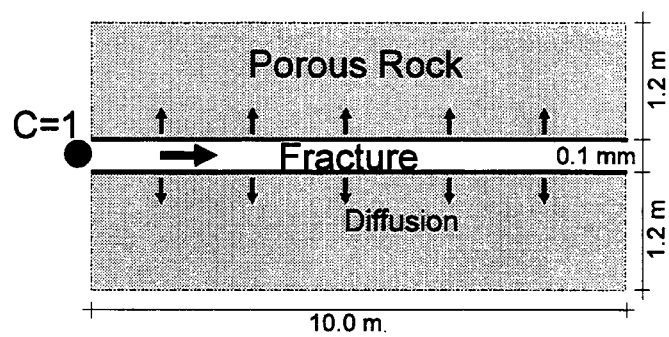

Fig. 3: Schematic description of Example 1

Figure 4 shows the simulation results compared to the results of the analytical solution of Tang (1981). The three curves exhibit concentration profiles along the fracture for three time steps: 97 days, 995 days and 9991 days. The solid curve represents the analytical solution, the square symbols indicate the TRIPOLY results at the nodes of the finite element mesh. Note that the original discretization is very course; original nodes are at locations 0.0 m, 0.1 m, 0.2 m etc. All the nodes in between the original ones have been added within the adaptive gridding procedure. The matrix blocks are discretized with 8 line elements.

As to the relatively simple geometry of this example, it is not possible to verify the codes ability to simulate diffusive transport in matrix blocks of complex shape. However, this has been successfully demonstrated in other studies (e.g. Birkholzer 1994). Here, our major goal is to check the performance of the Lagrangian-Eulerian scheme in combination with

the fracture-matrix interaction tool. Altogether, the analytical solution and the numerical results match quite well. There is evidence for certain numerical dispersion, especially for time step 9991 days. However, the spatial and temporal discretization is very coarse in our simulation. Much better results can be obtained by refining the original mesh.

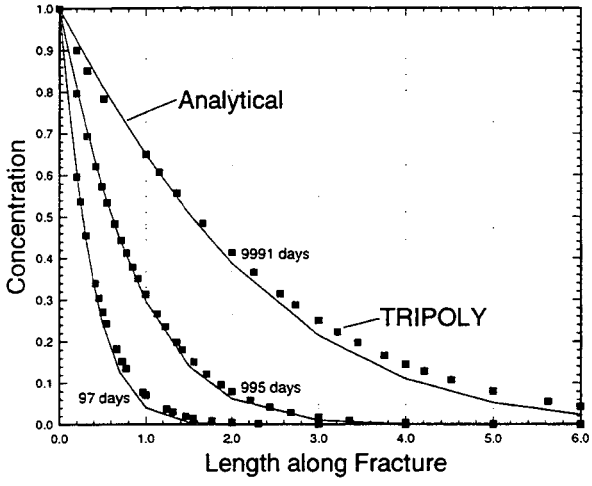

Fig. 4: Concentration along the fracture

6.2 *Transport in a complex fracture-matrix system*

The second example concerns advective-dispersive transport in a complex fracture network including diffusion into the porous matrix blocks. The fracture network of our example 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 5 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 no-flow boundary conditions are given at the upper and lower boundaries. The left boundary is associated with a hydraulic head of 0.1 m, the right boundary is associated with a hydraulic head of 0.0 m. We assume that the left boundary of the model area, which is initially clean, is contaminated with a Dirichlet-type boundary condition C=1. Solutes released at this boundary are carried through the model area and leave at the right (outflow) boundary.

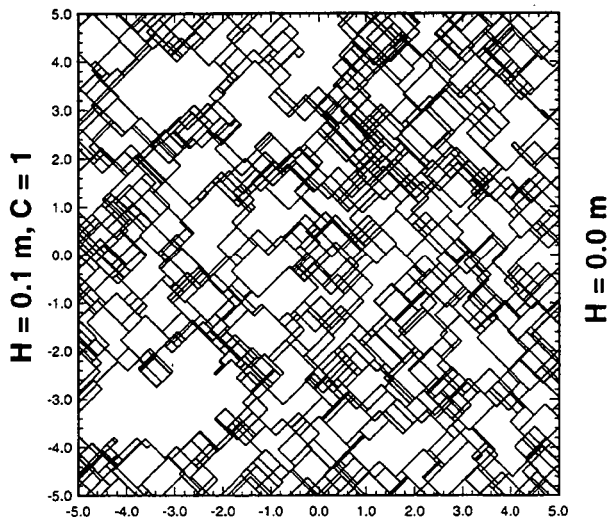

Fig. 5: Fracture network of example 2

Figure 6 shows the contaminant concentration in each matrix block at time 0.5×10^7 s. For the sake of visualization, average concentration were calculated out of the one-dimensional concentration profiles associated with each block. 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 is retarded and solutes in the fractures just begin to reach the outflow boundary at 0.5×10^7 s.

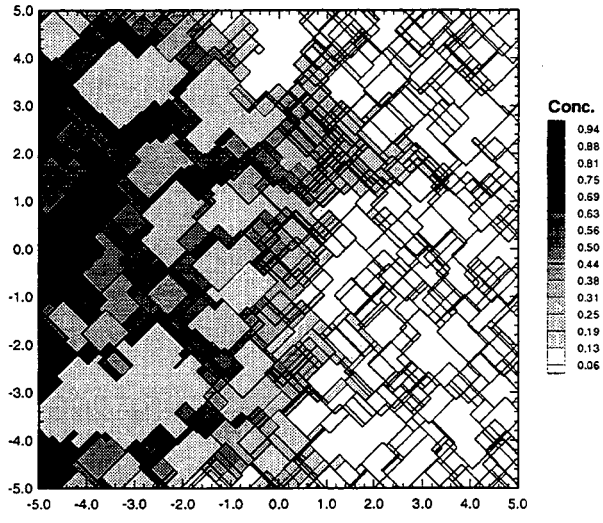

Fig. 6: Average concentration in the matrix blocks after 0.5×10^7 s

The contaminant build-up in the matrix is slower than in the fractures. Moreover, the concentrations in the blocks vary significantly, due to the different block sizes. Large blocks which offer a larger pore volume for storing contaminants are fairly clean whereas some smaller blocks are contaminated.

Results of another time step are presented in figure 7. After 3.0 x 10^7 s almost all of the fractures have concentrations values close to 1. However, the average concentrations of the matrix blocks show a different picture. Although many of the smaller blocks are already contaminated, there are a number of large blocks which are still fairly clean. This means that significant concentration differences between the fractures and the matrix can be obtained, and part of the solute diffuses from the fractures into the matrix pores. This process may continue for a long time because the diffusive transport in the matrix is very slow.

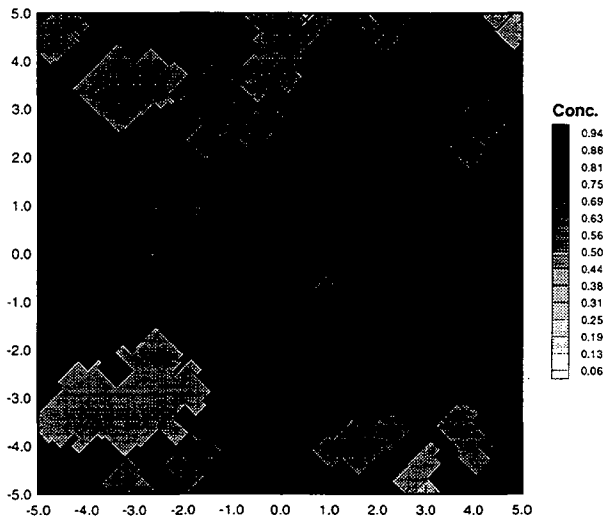

Fig. 7: Average concentration in the matrix blocks after 3.0 x 10^7 s

Figures 6 and 7 clearly demonstrate that the individual matrix blocks exhibit a very different response to perturbations in the fracture network, simply due to their variability in size and shape. This effect may even be enforced by spatially varying material properties. As presented in a companion paper by Jansen et al. (1996), the observed phenomenon has a strong impact on the assignment of equivalent continuum parameters for the matrix blocks, a problem which is associated with the use of dual-porosity models.

SUMMARY AND CONCLUSIONS

A new 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 porous 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.

ACKNOWLEDGMENT

This work was supported by a NATO-Postdoctoral Fellowship, provided by the German Academic Exchange Organization (DAAD), through the U.S. Department of Energy Contract No. DE-AC03-76SF00098. We would like to thank S. Finsterle and C. Doughty for thoughtful reviews.

REFERENCES

Bibby, R. 1981. Mass transport in dual-porosity media. *Water Resour. Res.* 17(4): 1075-1081.

Birkholzer, J. 1994. *Numerische Untersuchungen zur Mehrkontinuumsmodellierung von Stofftransportvorgängen in Kluftgrundwasserleitern.* Mitt. Inst. f. Wasserb. u. Wasserw. 93, Aachen: Academia.

Huyakorn, P.S., H. Lester, J.W. Mercer 1983. An efficient finite element technique for modeling transport in fractured porous media: 1. Single species transport. *Water Resour. Res.* 19(3): 841-854.

Jansen, D., J. Birkholzer, J. Köngeter 1996. Contaminant transport in fractured porous formations with strongly heterogeneous matrix properties. *Proc. NARMS '96*, Montreal.

Karasaki, K. 1986. *A new advection-dispersion code for calculating transport in fracture networks.* Lawrence Berkeley National Laboratory annual report LBL-22090, Berkeley, CA.

Neuman, S.P. 1984. Adaptive Eulerian-Lagrangian finite element method for advection-dispersion. *Int. Journal for Num. Meth. in Eng.* 20: 321-337.

Pruess, K., K. Karasaki 1982. Proximity functions for modeling fluid and heat flow in reservoirs with stochastic fracture distribution. *Proc. 8th Workshop Geotherm. Res. Eng.,* Stanford: 219-224.

Segan, S., K. Karasaki 1993. *TRINET: A flow and transport code for fracture networks - User's manual and tutorial.* Lawrence Berkeley Laboratory report, Berkeley, CA.

Tang, D., E. Frind, E.A. Sudicky 1981. Contaminant transport in fractured porous media: Analytical solution for a single fracture. *Water Resour. Res.* 17(3): 555-564.

Thomas, L.H. 1949. *Elliptic problems in linear differential equations over a network.* Watson Science Computer Lab., Rep. Columbia University, New York.

Ernest Orlando Lawrence Berkeley National Laboratory
One Cyclotron Road | Berkeley, California 94720

Prepared for the U.S. Department of Energy under Contract No. DE-AC03-76SF00098