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SCOPING CALCULATIONS FOR THE MULTIPLE WELL TRACER EXPERIMENT USING A VARIABLE APERTURE MODEL

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CALCULATIONS FOR TASK No 2.

Multiple Well Tracer Experiment (MWTE).

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ABSTRACT

Scoping calculations were made for the Multiple Well Tracer Experiment (MWTE) to be carried out in the Hard Rock Laboratory (HRL). Fractures are modeled as having variable apertures. Fluid flow and solute transport in the fractures are calculated. Diffusion into and sorption within the adjacent rock are also accounted for. Results from previous papers are summarized and discussed. These papers show that one or a few tests in a fracture do not suffice to characterize the properties of the fracture. Simulations for non-sorbing and sorbing tracers were also performed. Retardation for the sorbing tracers that diffuse into the rock matrix varies greatly in a same fracture. For the fast channels the retardation is small, whereas the slow channels show a large retardation. It is found that it is not possible to characterize the variable properties of the fracture by a small set of simple hydraulic and tracer tests, if the results are to be used for extrapolation in time and space.

CONTENTS

SUMMARY

Scoping calculations were performed for the Multiple Well Tracer Experiment (MWTE). MWTE is one of the experiments planned in the Hard Rock Laboratory (HRL). A large number of boreholes are drilled to intersect a single fracture. Hydraulic and tracer tests will be made by using these boreholes. The objective of the MWTE is to test the validity of different conceptual and numerical models of solute transport in single fractures and to discriminate between them.

In these calculations the single fracture is modeled as having a variable aperture. The local apertures are taken from a log-normal distribution with a specified mean and standard deviation. The apertures are correlated in space. Fluid flow and solute transport in the fracture are calculated. Solute transport is calculated by using a particle-following technique. Diffusion into and sorption within the adjacent rock are also accounted for. Local hydrodynamic dispersion in the fracture is neglected, but on a larger scale there is dispersion due to the local velocity variations.

Results from previous papers are summarized and discussed. Solute transport in a fracture with a variable aperture shows some anomalous features. Breakthrough curves from tracer tests are primarily determined by the spatial variability in fracture aperture, the location of the injection and the injection flow-rate used. Moreover, tests performed with variable injection flow-rate may be very difficult to analyze. These papers show that one or a few tests in a fracture do not suffice to characterize the properties of the fracture.

Simulations for non-sorbing and sorbing tracers were performed. Water was pumped up in the centre of a fracture and tracers were injected at a specified distance from the centre. The results are presented qualitatively as flow paths, mass flow, concentration patterns and breakthrough curves. The fluid is found to flow into the withdrawal hole through a few channels. The mean travel time and dispersion of different runs vary within a wide interval. Retardation for the sorbing tracers that diffuse into the rock matrix also varies greatly in the same fractures. For the fast channels the retardation is small, whereas the slow channels show a large retardation.

We find that it is not possible to characterize the variable properties of the fracture by a small set of simple hydraulic and tracer tests, if the results are to be used for extrapolation in time and space.

1 INTRODUCTION AND BACKGROUND

In the Hard Rock Laboratory (HRL), various types of experimental projects have been planned. One of these is the project Flow and Transport Processes in the Detailed Scale. The tests in this project are organized into three sub-projects:

- Pore volume characterization, where grout, epoxy resin, dyes, or the like are injected into a fracture that is later excavated by drilling.

- Multiple well tracer experiment, where a large number of boreholes are drilled to intersect a single fracture. Cross-hole hydraulic and tracer tests are made to characterize flow and transport in the fracture plane under different boundary conditions.

- Matrix diffusion experiment, where sorbing tracers with different sorption capacities are injected for a long time into a permeable fracture. After injection has stopped, a dye or resin is injected into the fracture to mark the flow paths. The fracture is excavated to observe the distribution of flow paths and penetration of tracers into the rock matrix.

Scoping calculations on the Multiple Well Tracer Experiment and the Matrix Diffusion Experiment were proposed to the Äspö Task Force on groundwater flow and transport of solutes. In this paper, scoping calculations for the MWTE are presented. The scoping calculations should provide input for specifying the MWTE geometry, borehole configuration and distance between boreholes, as well as the transmissivity of the target fracture.

Before we present the scoping calculations, results from previous calculations will be discussed in relation to the MWTE. These calculations are based on a model where the fracture is considered as a having variable aperture (Moreno et al. 1988). The implications of the variable aperture on the proposed tracer tests will also be discussed. From these results, we could point out that situations in which scoping calculations were meaningful.

2 DESCRIPTION OF EXPERIMENT

The main objectives of the project "Flow and Transport Processes in the Detailed Scale" are: to improve understanding of transport processes, to determine *in-situ* parameters for transport of sorbing nuclides in a single fracture and to quantify variability in flow and transport parameters for fractures of different characters. The project is expected to provide data for testing, and to refine the models used for transport of radionuclides in fractured rock.

2.1 Multiple Well Tracer Experiment (MWTE).

The objective of the Multiple Well Tracer Experiment is to test the validity of different conceptual and numerical models of tracer transport in single fractures. The experience obtained is expected to facilitate discrimination between different models or to provide bounds for where models give reasonable approximations.

The MWTE is designed to study transport processes in a single transmissive fracture. The basic concept of the experiment is that significant transport parameters may be evaluated from cross-hole tracer and hydraulic tests in the same fracture under different boundary conditions. Some characteristics of the planned tests and its motivation are:

- A large number of boreholes intersecting the fracture, to evaluate effects of scale and flow direction, longitudinal and transverse dispersivities.

- The use of different boundary conditions, to evaluate the importance of flow velocity on dispersion.

- The use of different tracers, to evaluate sorption effects (conceivably, matrix diffusion).

In a tracer test with an injection and a recovery point, the transport of the tracer is constrained by the flow field. Tracer tests will be performed with injection and retrieval flow-rates, that cause a significant disturbance to the natural flow field in order to obtain data on the constraints set by the flow field. This puts a upper limit on the tracer recovery that may be obtained. Different injection rates will be used to assess the dependence of velocity on dispersion. Dispersion is observed by sampling of tracer in boreholes situated between the injection and retrieval points, as well as on both sides of the direct flow paths.

A number of boreholes are drilled to intersect a "single" fracture. A central borehole surrounded by two circles of six boreholes is proposed in the tentative design. The diameter of the outer circle was set to 5 metres, and the transmissivity for the target fracture is assumed to be 10^{-8} m^2/s.

Cross-hole tracer tests and hydraulic (single-hole and cross-hole) tests will be carried out in the same fracture under different boundary conditions.

For the MWTE, scoping calculations will be made to determine suitable properties of a target fracture, the number of boreholes, and dimensions of the borehole array.

2.2 Possible problems in these experiments

In the test plan for flow and transport processes in the detailed scale for the MWTE (Olsson, 1992), the following possible problems are discussed:

- To identify what effectively is a single fracture. Intersecting fractures with non-negligible conductivity are likely to be present and have to be included in the experimental set-up. Permeable fractures will be monitored during testing.

- With pronounced channeling, some boreholes may be not transmissive, thus limiting the number of active boreholes. Moreover it will be difficult to recognize the fracture plane as a transmissive feature, as only a few of the boreholes are expected to have measurable transmissivities.

3 THE MODEL

In the analysis of tracer tests in fractured media, a discrete representation of the fractures has often been used. These fractures are then represented by a pair of parallel plates with a constant aperture. Theoretical and experimental studies on single fractures, however, showed the parallel-plate representation of the single fracture to be inadequate in the description of fluid and tracer movement through a fractured medium (Moreno et al., 1988).

Field experiments of flow and solute transport in individual fractures in granitic rocks showed that flow is very unevenly distributed along the fracture planes, and that large areas did not carry any water (Abelin et al., 1985; Neretnieks, 1985; Bourke, 1987). One attempt to account for the obvious "channeling" effects was to assume that flow takes place in independent channels. This has been modeled as flow in a number of independent channels with different apertures (Neretnieks et al., 1982; Moreno et al., 1985) which has lead to the development of a model where the aperture varies stochastically in the fracture.

In earlier papers (Moreno et al., 1988, 1990; Moreno and Tsang, 1991), a two-dimensional model of a fracture with variable apertures has been presented. Flow and solute transport calculations in the fracture were made with this model. The model allows for point tracer injection and withdrawal in the two-dimensional fracture plane. The results for flow in two dimensions showed that fluid flows very unevenly in a single fracture and that it takes place in preferred paths. A number of anomalous features of tracer transport were identified and discussed.

One of the most important retardation mechanisms for radionuclides is the diffusion into the rock matrix from the mobile water in the fracture. We have therefore incorporated this effect in our model. It adds a new dimension to the transport process because the solutes now also have access to the inner porosity of the rock matrix and the inner sorption sites. Our model thus has two dimensions in the fracture plane and one in the rock matrix.

3.1 The conceptual model

The fracture surfaces are rough, and thus the aperture is not constant and varies spatially. The spatial variation of the fracture aperture is characterized by a spatial correlation length. This means that within a range smaller than the correlation length the aperture values are more likely to be similar, but at separation distances much longer than the correlation length there is little or no correlation between apertures values. The apertures in the fracture may be defined by an aperture density distribution, $n(\delta)$, and a spatial correlation length, λ. The extent of the fracture in x and y directions is L_x and L_y.

Now let us assume there is a parallel regional flow in the plane of the fracture, i.e. that two opposite ends of the fracture have a constant hydraulic head difference. Fluid flowing through the fracture seeks out the least resistive pathways. The main flow is expected to occur through a few channels in the fracture plane. "Channels" means the preferred flow paths in the fracture. If the direction of the pressure gradient is changed, a new set of channels would be obtained. Zones with small apertures will usually have very little flow. Zones with large apertures do not, however, necessarily have a large flow, because they may be isolated from the main flows by nearby constrictions in the fracture.

For a fracture with an overall flow under a "regional" pressure gradient, a solution containing the tracer may be injected at a point in the fracture plane. The injection pressure modifies the previously existing fluid flow pattern around the injection point. For a given configuration of the variable apertures, the injection flow-rate feeds the tracer into paths that are available for transport. The larger the injection flow, the larger the number of paths that may be reached by the tracer. However, the pattern of the flow paths depends strongly on the variable apertures near the injection point.

The formulation of the model is taken from Moreno et al. (1988, 1990). The fracture plane was partitioned by grids with a different aperture assigned to each node enclosed by grid lines. For the present study, the grid is 100 x 100 nodes. A log-normal distribution for the variable apertures in the plane of the single fracture, and an exponential function for the spatial covariance of the apertures, were chosen.

3.2 Fluid flow calculations

For laminar flow conditions the volumetric flow rate through a channel of constant aperture may be written as (Bird et al., 1960):

$$Q = \frac{\delta^3}{12\,\mu} W \frac{\Delta P}{\Delta L} \tag{1}$$

where δ is the channel aperture, μ the dynamic viscosity, W the width of the channel, and $\Delta P/\Delta L$ the pressure gradient. We assume that the apertures are very much smaller than the flow distance in the nodes, so that the influence on pressure drop by the diverging or converging parts of the flow path is negligible. The flow between two adjacent nodes is determined by both apertures. The flow between nodes i and j may be expressed as:

$$Q_{ij} = \frac{1}{6\mu}\left[\frac{1}{\delta_i^3} + \frac{1}{\delta_j^3}\right]^{-1} \frac{\Delta y}{\Delta x} (P_i - P_j) \tag{2}$$

where Δx is the node length in the direction of the flow and Δy its length in the perpendicular direction.

The mass balances at each node may be written as:

$$\sum_j Q_{ij} + I_i = 0 \tag{3}$$

where Q_{ij} is one of the flows coming into or going out of node i. I_i is injection into or withdrawal from node i. We assumed that the injection and the withdrawal are carried out in the centre of the respective nodes.

The solution of this system of equations yields the pressure at each node. The flow rate between adjacent nodes may then be calculated.

3.3 Calculations of solute transport in the fracture

The residence-time distribution of the solute, RTD, is often described by two quantities which are of interest for solute transport: the mean residence time and the variance of residence times. There are several mechanisms which may cause the spreading of a species transported by a fluid. In this context, we consider only velocity variations between the different channels. Other effects such as molecular diffusion, hydrodynamic dispersion, matrix diffusion, etc. will be discussed later. We also assume that local longitudinal dispersion within each node is negligible and that the overall dispersion in the fracture is caused by the different residence times along different pathways only.

The solute transport is simulated using a particle-following technique (Schwartz et al., 1983; Robinson, 1984; Moreno et al., 1988). A given number of particles is introduced in the flow field at the injection node. Each particle is followed along its path, from the injection to the collection point through the intersections (Hull et al., 1987; Philip, 1988). There are different ways to carry out this particle following with respect to the dispersion of the particles. We will use a method which includes mixing of the tracers only in the paths (branches) between two intersections, and no mixing at the intersections (Moreno et al., 1990).

The residence time in a given node or channel for non-sorbing tracers is determined by the total flow through the node and its volume. The residence time of an individual particle along the whole path is determined as the sum of residence times in every channel that the particle has traversed. The residence time distribution is then obtained from the residence times of a multitude of individual particle runs.

From the distribution of the residence times, the mean residence time and variance may be calculated. The mean residence time, t_w, and variance, σ_t^2, may be used to determine the Peclet number, which is a dimensionless measure of the dispersion of the tracer. The Peclet number, Pe, is calculated as (Levenspiel, 1972):

$$\frac{2}{Pe} = \frac{\sigma_t^2}{t_w^2} \tag{3}$$

where σ_t is the standard deviation of the residence times, and t_w is the mean.

3.4 Diffusion into the matrix

For the water residence time, we tend to think only of the residence time of the water that flows in the aperture(s) of the fracture. The rock matrix is, however, porous and contains stagnant water. As this does not flow, it is traditionally not included in the hydraulic (flow) models. When contact times between the flowing water in the fracture and the porous rock are long, the water molecules in the rock and those in the fracture are exchanged by molecular diffusion. For very long periods of time, the stagnant water will be fully available to "flow." This may be studied by a tracer which diffuses into and out of the matrix. For "fast" flow, only the water volume in the fracture, V_f, will contribute to the residence time. For very slow flow, both the water in the fractures and in the rock matrix, V_m, will contribute to the residence time. In the first case the residence time is $t_f = V_f/Q$, in the second case it is $t_{fm} = (V_f + V_m)/Q$. In crystalline rocks of interest (Abelin et al., 1991; Birgerson et al., 1992) $V_m >> V_f$ and thus may dominate the residence time. For intermediate times, only a fraction of V_m is accessed by diffusion.

These effects are even more important for sorbing tracers. The matrix diffusion effect is therefore included in our model, and we will show that it may influence the experiments under some circumstances.

When dispersion in the paths and/or diffusion into the rock matrix are considered, different particles in the same paths will have different residence times. Here, residence times for the particles may be described by the RTD of the particles, expressed as a probability density function, pdf. It may be thought of as the outlet concentration for a pulse injection. If this curve is integrated over all the possible residence times, the cumulative distribution of the residence times is obtained.

When diffusion from the moving water into and out of the rock matrix takes place, a particle may reside in the matrix for some time, in addition to its residence time in the water in the channel member. For a flat channel from which the diffusion is perpendicular to the channel surface, a simple analytical solution is available for the RTD. The cumulative curve, F, for the residence times is obtained as (Carslaw and Jaeger, 1959):

$$F = \operatorname{erfc}\left(\frac{(D_e K_d \rho_p)^{0.5} t_w}{(t - R_a t_w)^{0.5} \delta}\right) \qquad (4)$$

for times greater than the water-plug-flow residence time t_w. Otherwise the value is zero. Equation (4) considers only advection in the channel and diffusion into the rock matrix. Longitudinal dispersion is neglected. In Equation 4, D_e is the effective diffusion coefficient, K_d the volume sorption constant, ρ_p the bulk density of the rock, and R_a the surface retardation factor.

For a rectangular channel, the water-plug-flow residence time is obtained from the ratio between the channel volume and the flow rate through it. It may be calculated by LWδ/Q. Introducing this expression into Equation (4) yields:

$$F = \text{erfc}\left(\frac{(D_e K_d \rho_p)^{0.5} L W}{(t - R_a t_w)^{0.5} Q}\right) \qquad (5)$$

For particle following, we use the same technique as Yamashita and Kimura (1990). The travel time for each particle in a channel member is determined by choosing a uniform random number in the interval [0,1]. The travel time for the particle, t, is then calculated by solving for t in Equation (6):

$$[R]_0^1 = \text{erfc}\left(\frac{(D_e K_d \rho_p)^{0.5} L W}{(t - R_a t_w)^{0.5} Q}\right) \qquad (6)$$

4 RESULTS FROM PREVIOUS CALCULATIONS

In earlier papers, some features of fluid flow and solute transport arising from fracture aperture variability were studied (Moreno et al., 1988, 1990; Moreno and Tsang, 1991). It was found that if a pressure gradient is imposed in the fracture, and the fluid flow is calculated, fluid flow occurs predominantly in a few preferred paths. The flow rates between nodes vary by several orders of magnitude. Figure 1 shows the flow rates calculated for a fracture, with a standard deviation in fracture aperture of 0.5 (in base 10 logarithm) and a correlation length of 0.1 L. The results show a strong channeling effect; the fluid seeks the less resistive paths in the fracture. The density of these channels is related to the correlation length used in the generation of the fracture apertures. For a small correlation length, the channels are closer to each other (Moreno et al., 1988). Some results obtained in these papers are presented below.

Hydraulic conductivity measurements were simulated on many realizations of fractures with variable apertures. Water was injected in several locations of the fracture, one location at a time, with a given flow rate. The local hydraulic conductivity was determined from the pressure needed to reach this flow rate . It was found that the local hydraulic conductivity may vary by several orders of magnitude. These large variations are also observed in some field tests. This indicates that a few local hydraulic conductivity measurements in a heterogeneous system, such as the variable aperture fracture, may not give the needed information (Moreno et al., 1990).

4.1 Solute transport; influence of the injection flow-rate and location.

Tracer tests are commonly performed to investigate transport properties (e.g., dispersion, flow porosity, etc.). For flow in a single fracture, an average fracture aperture and the dispersion (often expressed as the Peclet number) are the entities commonly sought. In most tracer tests, the water flow may be thought of as a parallel regional flow or as radial convergent flow. We will discuss both modes.

For the parallel regional flow, tracer tests were simulated in a fracture with flow from one side to the opposite side. Tracers (or particles) are injected at a given location in the fracture and collected in several sections at the outlet side. Different injection flow-rates are used. Figure 2 shows the tracer paths for two injection flow-rates, 0.01 and 0.10 of the total flow rate in the fracture.

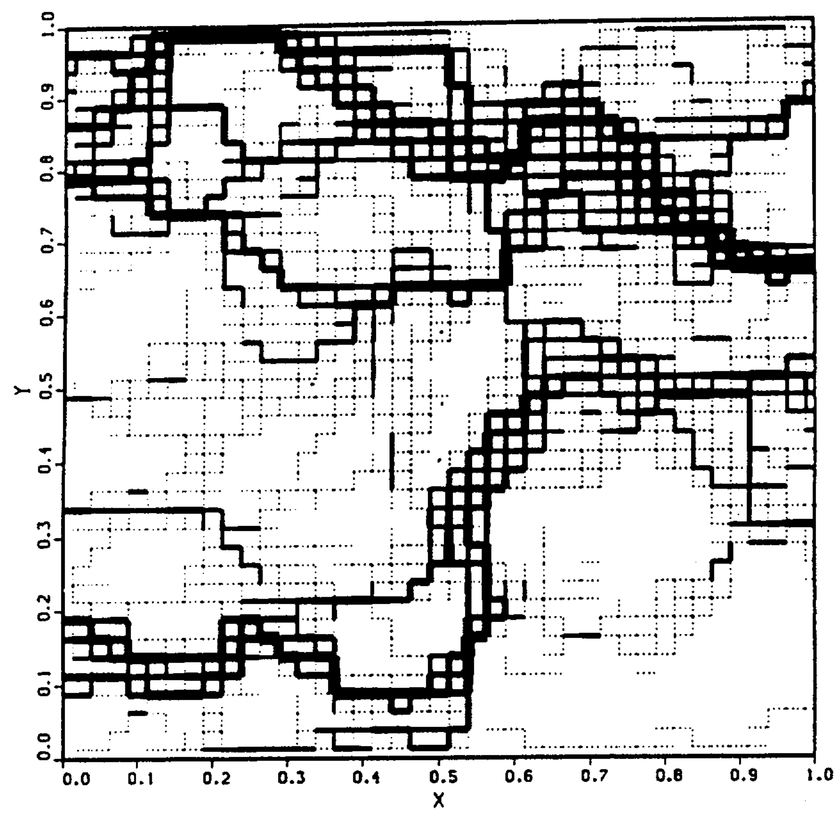


Figure 1. Fluid flow in the fracture for parallel fluid flow from left to right. The line thickness is proportional to the square root of the flow. Flow rates less than 0.2 % of the total flow are not drawn.

In these simulations, it was found that when a small injection flow-rate is used, most of the tracer could flow through one or few paths, but for large injection flow-rates the tracers use more paths. This implies that residence time and dispersion of the tracer are increased. Thus, tracer tests with variable injection flow-rates may be very difficult to analyze, owing to changes in the residence time and dispersion of the tracer with time, because different sets of pathways are sought out by the tracers during the experiment.

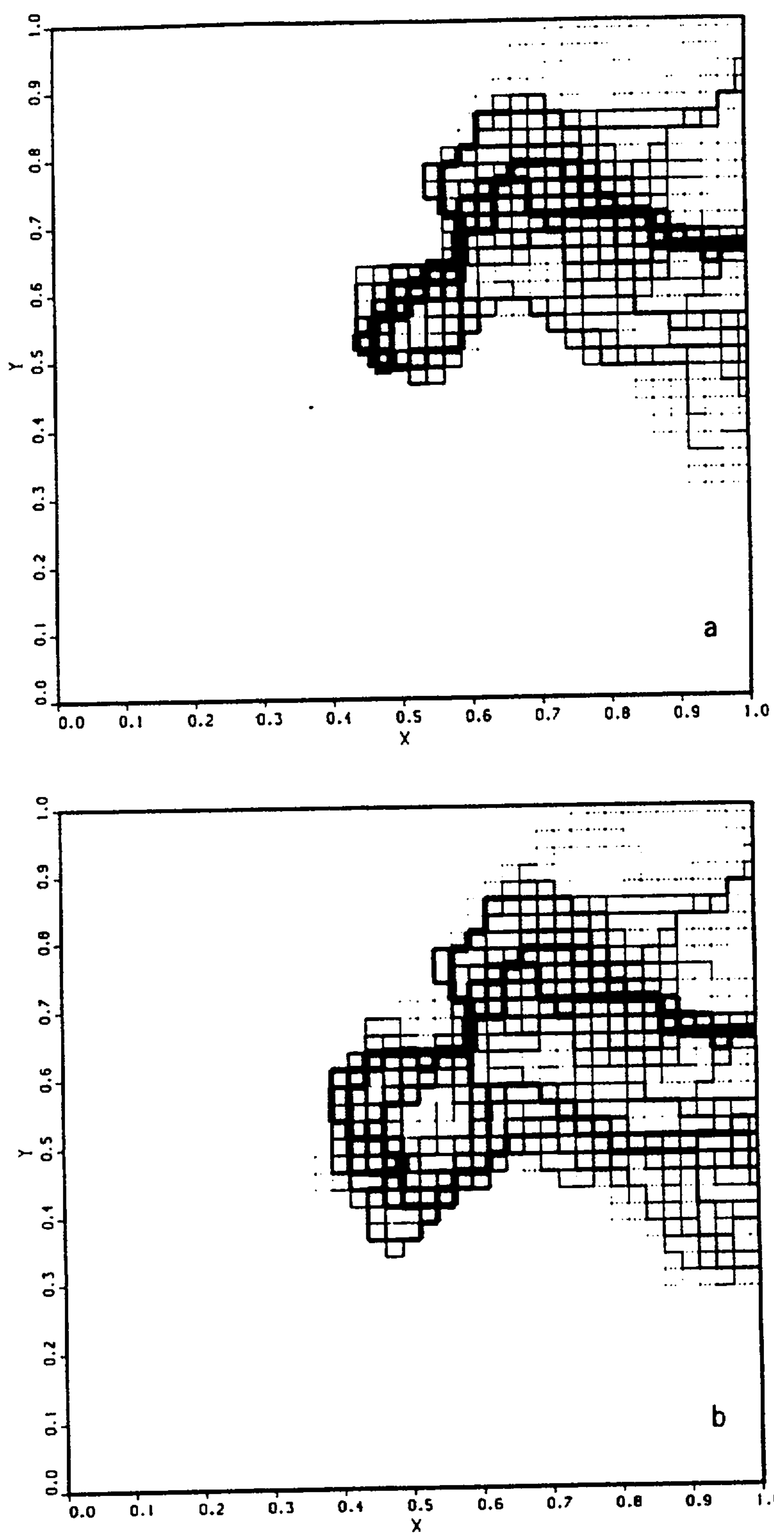


Figure 2. Tracer path for parallel flow with injection flow-rates of a) 0.01 and b) 0.10 of the total flow rate in the fracture at the location (20,20). The line thickness is proportional to the square root of the number of times that particles pass through a connection.

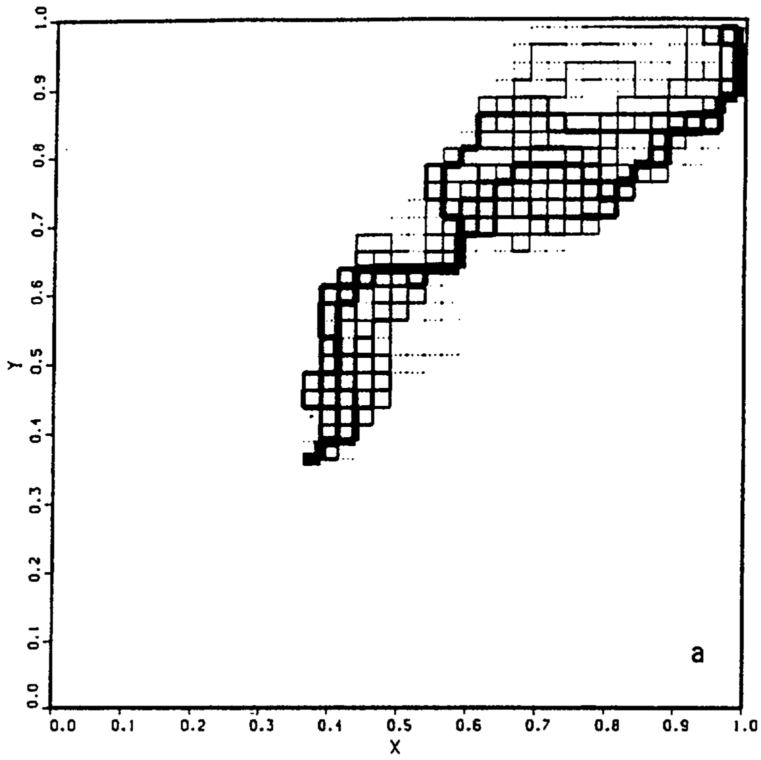
It should be noted that a negligible injection flow-rate may result in a substantial increase in the residence time. This effect may be found in field experiments when a very small flow is used for the injection of the tracer, with the purpose of not disturbing the "natural" flow which existed before the injection. If the injection point happens to be located in an area with low flow and quite a large volume, it will take the tracer a very long time to travel out to the mainstream of the flow field.

Results also show that the residence times and dispersion obtained in a specific tracer test may vary considerably. Thus the characterization of the transport properties of the fracture is made with a very high uncertainty if tracer experiments are performed with only one or a few injection points. The results depend on the injection location, the injection flow-rate, and the location of tracer collection.

For tracer tests in a fracture with a regional convergent flow, the situation is similar. We will discuss some results of simulations using a convergent flow system, because *in-situ* tracer tests are often carried out by withdrawing water from a borehole. This creates a convergent flow field toward a sink into which tracers injected at another point flow. The injection flow-rate is often small, but not always negligible compared to the total flow into the collection borehole. In these simulations (Moreno et al., 1990) injection flow-rates in the interval 0.005 to 5.0 % of the production flow-rate at the collection point were used.

Tracer flow paths for two injection flow-rates are shown in Figure 3. For the larger injection flow-rate the injection zone was much greater than when a smaller injection flow-rate was used. Thus an increase in the injection flow-rate increased the tracer residence time. The dispersion greatly increased with an increase in the injection flow–rate, which implies the increased involvement of many more flow paths to the collection point, compared to the situation with a low injection flow-rate. When the injection flow rate was increased from 0.005 to 0.05 of the withdrawal flow-rate the tracer residence time increased from 0.43 to 0.93 time units and the Peclet number changed from 70 to 2.5.

The results of the tracer simulations show that residence times vary over a wide range. The residence times depend on the injection flow-rate and where the tracers were injected. If these residence times are used to calculate the fracture aperture, very different apertures will be found. The large differences between fracture apertures are critical when these aperture values are used to characterize the fracture, and indicate the need for great care in the analysis and interpretation of field test data.



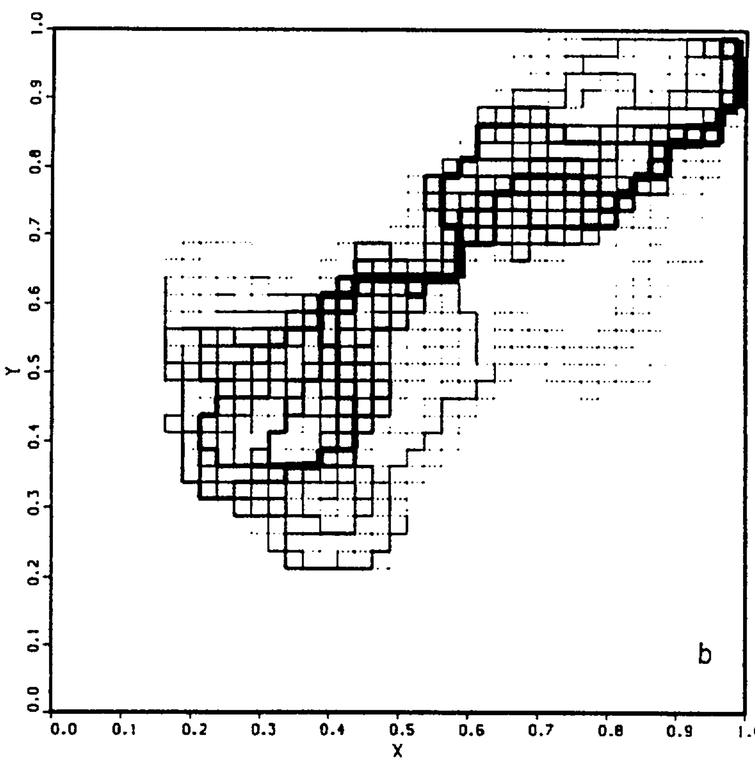


Figure 3. Tracer path for convergent flow with injection at location (15,15). The tracer injection flow-rates are a) 0.005 and b) 0.05 of the withdrawal flow–rate. The line thickness is proportional to the square root of the number of times particles pass through a connection.

When the injection was carried out at a location with a good connection, the injection flow-rate used had little influence on the breakthrough curve obtained. On the other hand, for injections at a location with a bad connection with the production point, the influence of the injection flow-rates on the breakthrough curve was large.

The uncertainty of the results from this kind of tracer test is very large. The values depend on the location of the injection hole and collection hole, and also on the injection flow-rate. In general, if the injection is carried out in a zone directly connected to the collection hole, the resulting "mean aperture" may be smaller than the actual mean aperture, and the influence of the injection flow-rate will be small. If the injection occurs at a location not directly connected to the collection hole, the aperture will seem to be very large, and to be strongly influenced by the injection flow-rate.

It may be concluded that, because of the stochastic nature of fracture apertures, one–point tracer tests in a fracture are not sufficient to characterize the hydraulic properties of the fracture (conductivity, aperture, and dispersivity). The dispersivity determined in these simulations may vary by one to two orders of magnitude. If fracture apertures are calculated, they may also vary by some orders of magnitude. The variation in the dispersion and residence time with the injection flow-rate complicates the interpretation of tracer tests performed in fractures.

4.2 Discussion of these results and implications for tracer tests.

The results presented above point out some of the difficulties that may be found in the analysis of tracer tests in fractured rocks. Two different geometries were studied: the parallel and the convergent flow. The conclusions are similar for both. The breakthrough curves are primarily determined by the spatial variability in fracture aperture and the location of the injection point within the aperture field. In practice, we do not have *a priori* information to decide where the borehole should be drilled. After the borehole has been drilled, the determination of hydraulic conductivity and interference tests may improve our knowledge of the fracture around the injection hole.

The results also show that, in certain cases, the injection flow-rate may strongly modify the breakthrough curves obtained in tracer tests. For an *in-situ* tracer test where the injection rate changes, the analysis of the results may be very difficult, if not impossible. Variation of the injection flow-rate may modify the path of the tracer through the fracture. The injection flow-rate also influences the dispersion, since a large injection flow-rate creates new pathways that results in an increase in the dispersion.

The use of very small injection flow-rates, or pulse injection with a small injection volume, may present an even larger problem. If the tracer is injected in a location with a small flow rate and a large volume, the residence time for the tracer in the fracture may be very large. Low flow does not imply small apertures, but only that the injection point is hydraulically poorly connected to its neighbours. This is often not found *a priori* by pressure tests, since the hydraulic connection may be a function of local pressure. In other words; with an applied pressure at this location, connection with the withdrawal hole may be obtained by seeking other paths (e.g., moving first in the opposite direction).

The problem caused by a small injection flow-rate cannot be avoided by using a large injection flow-rate. Here, if the injection occurs at a point with a poor connection to the collection point, the breakthrough curve will show large residence times and high dispersion. This is because the tracer seeks new paths in the fractures. On the other hand, injection at points with a good connection with the collection hole and large flow may yield short residence times and smaller fracture apertures.

From the simulations we may conclude that, because of the stochastic properties of fracture apertures, one or a few tracer tests in a fracture is not sufficient to characterize the hydraulic properties of the fracture (e.g., conductivity, aperture, and dispersivity). Tracer tests made in different ways and along different paths will give different results even of mean properties.

5 SIMULATED CASES

Above, we showed some of the general characteristics of fluid flow and solute transport in a fracture with a variable aperture. Here, some specific simulations are made for the Multiple Well Tracer Experiment.

First, we discuss tracers that do not have access to the matrix porosity. In the model, the transport of tracers that do not interact with the matrix (non-interacting tracers) is independent of the duration of the experiment. If the time is normalized, for example, with respect to the mean residence time, the same breakthrough curve is obtained, regardless of the pumping flow-rate. For tracers that interact with the matrix, the situation is different. The impact of matrix diffusion is strongly influenced by the contact time between the tracers and the matrix. For short travel times, the impact of matrix diffusion may be small.

For these reasons, the size of the fracture and the pumping flow-rate have to be specified in the simulations. The fracture we use is a square with six-metre sides. Different flow rates are used for the pumping flow in order to cover small and large impacts of matrix diffusion.

The situation where water is pumped up in the centre of the fracture and the tracer is injected in a hole at a given distance from the centre is simulated. The distance between the injection and the withdrawal hole is 1.8 m. In the same fracture, eight locations are used for the injection hole. The boundary conditions are: a specified head at the four sides and given withdrawal and injection rates. Figure 4 shows a schematic diagram of the fracture and location of the injection holes used, as well as the boundary conditions.

In a first set of simulations, tracers that do not interact with the matrix are injected. Two different injection rates are used. For these tracers, only the ratio between injection and withdrawal flow-rates is important, as discussed above.

In a second set of simulations, tracers that may diffuse into the rock matrix are injected. Equation 5 points out that the rate of transport of a tracer that diffuses in the matrix is determined by the factor:

$$\frac{(D_e K_d \rho_p)^{0.5} L W}{Q}$$

So an increase in the flow of a factor of two, for example, has the same effect as a decrease in the diffusion or sorption coefficient of a factor of four. This is valid for the situation where diffusion into the matrix is important, because the transport time for a non-active tracer (without diffusion) is then negligible with respect to the time of interest in our calculations.

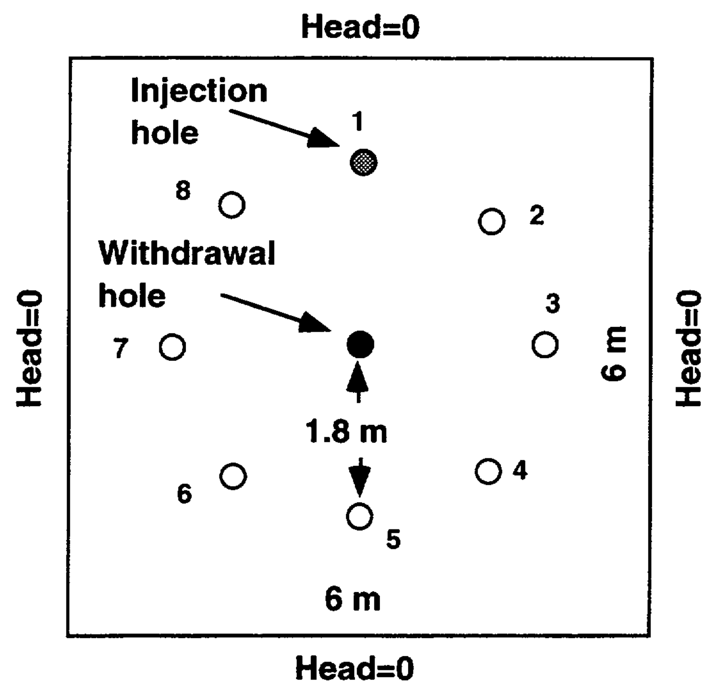


Figure 4. Schematic diagram of the fracture with injection and withdrawal hole, and boundary conditions.

6 RESULTS OF THE SIMULATED CASES

Fluid flow paths, tracer mass flow-paths, concentration patterns and breakthrough curves are studied. Density plots are used to visualize the patterns. For all patterns a white node means that the value is zero or very small. A black node means a high value of the parameter (flow, mass, or concentration).

In these simulations, the mean aperture of the fracture is chosen to be equal to 0.1 mm and the standard deviation in the aperture distribution to be 1.2 (natural logarithm). A correlation length of 0.3 m is used. The pumping flow-rate used is 10 ml/h. This means that the mean residence time would be 101 h if the fracture had a constant aperture of 0.1 mm.

The fracture is created by a stochastic process. The results for a given fracture correspond to only one of the infinite number of possible realizations.

The head is the same at the four boundaries. Then the injection is made with a very small flow rate compared to the pumping flow-rate in the centre of the fracture (0.001 – 0.01 times the pumping flow-rate). Figure 5 shows the flow paths. Pronounced channeling is observed. Most of the fluid flow into the withdrawal hole is through only five or six channels.

6.1 Tracers that do not interact with the matrix

Tracers are injected in one of the eight possible injection holes, one location at a time. Figure 6 shows the mass flow and concentration in the fracture when the tracer is injected in location # 3 (see Figure 4). From the flow paths, it may be seen that this injection occurs in a location with a good connection with the withdrawal hole. Here, the influence of the injection flow-rate is not important. It may also be observed that the tracer does not go directly to the withdrawal hole. Most of the tracer first goes downwards and then turns up following the flow channels. The concentration decreases rapidly with the distance to the injection hole, due to the mixing with water from other locations.

Figure 6 also shows that if detection holes are used to study transverse dispersion, very different values may be obtained. For example, if a detection hole is located some decimetres below the line that connects the injection and withdrawal holes, a very large transverse dispersion would be obtained. On the other hand if the detection hole is located above the line, the transverse dispersion would seem to be very small.

Table 1 shows the local flow caused by withdrawal pumping and the transmissivity at the different injection locations. From the travel time distribution for the particles the mean residence time and the dispersion (Peclet number) are evaluated. The results are shown in Table 2. The mean travel times are found in a quite wide interval. The dispersion of the tracer is very different. Breakthrough curves with very large dispersion (Pe about 7) and with quite small dispersion (Pe 150–200) are found. Figure 7 shows breakthrough curves for three of the tracer tests shown in Table 2. These Peclet numbers are higher than what is commonly found in field experiments, typical values are in the range 1-10 (Abelin et al., 1991; Birgerson et al., 1992). We have found, however, that if we include matrix diffusion in our simulations, with porosity and diffusivity values representative of Sweden crystalline rocks, the dispersion increases significantly. Peclet numbers then range from values less than 1 to 7.

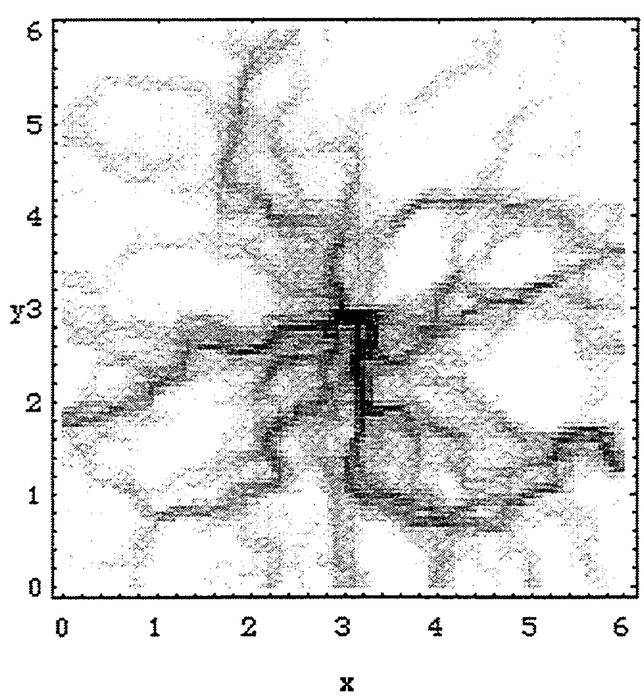


Figure 5. Flow paths for withdrawal hole located at the centre of the fracture and constant head at the four sides.

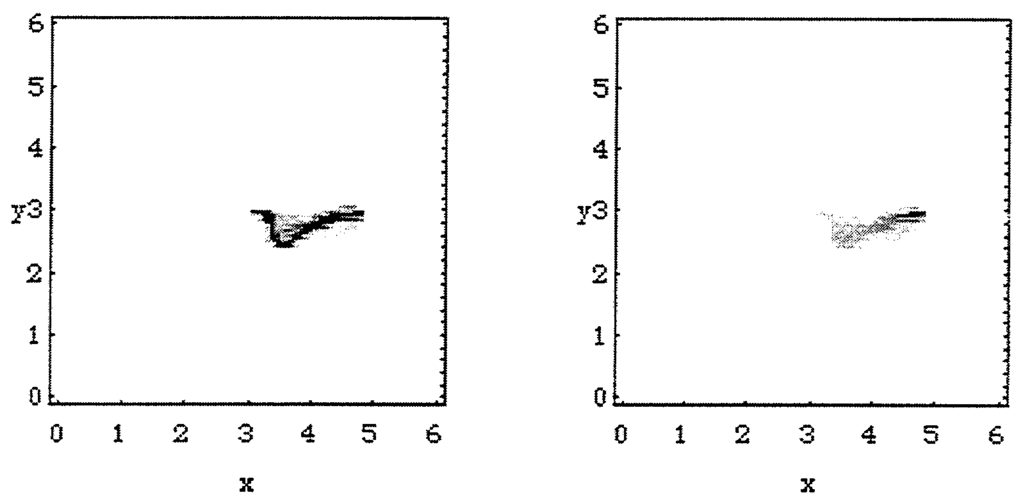


Figure 6. Mass flow (left) and concentration (right) for the same situation shown in Figure 5. Injection hole is at location # 3.

Table 1. Local flow caused by withdrawal pumping and transmissivity at the different injection locations. Values relative to the value at the injection hole # 1

Injection location	Relative transmissivity	Local flow caused by withdrawal pumping
1 *	1.00	1.00
2	1.19	0.02
3	1.79	0.16
4	0.59	0.76
5	12.20	0.06
6	5.11	0.09
7	0.29	1.24
8	1.06	1.32

* Normalizing point

Table 2. Mean residence time and Peclet number for tracer injection in eight different locations.

Injection location	Mean residence time (h) ratio injection to withdrawal rate 0.001	0.01	Peclet number ratio injection to withdrawal rate 0.001	0.01
1	122	122	16.3	14.4
2	301	257	13.1	11.5
3	311	229	82.2	51.2
4	96	100	45.3	28.2
5	120	92	6.7	5.1
6	137	149	192.4	27.3
7	99	98	126.6	106.5
8	61	59	7.5	7.7

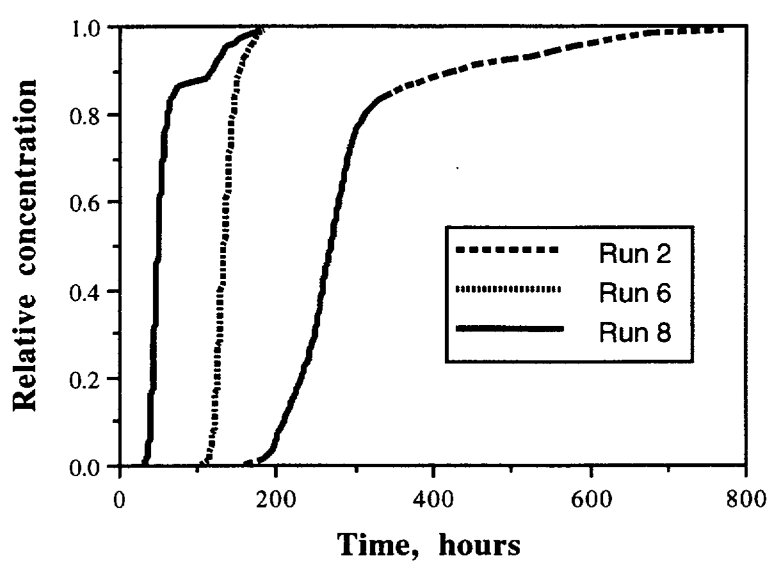


Figure 7. Breakthrough curves for some runs shown in Table 1, for a tracer that does not interact with the matrix.

6.2 Tracers that interact with the matrix

For tracers that diffuse in the rock matrix and also may be sorbed within the matrix, the properties of the rock matrix have to be known. A value of $2.0 \cdot 10^{-13}$ m^2/s is used for the effective diffusion coefficient. The sorption coefficient of the rock corresponds to a tracer weakly sorbed in the rock. The product K_d ρ_p used is 1.0 m^3/m^3. Surface sorption is not accounted for.

The injection of the tracer is carried out in the same locations as where the non-interacting tracers were injected. The breakthrough curves are shown in Figure 8, for the same runs as shown in Figure 7 when diffusion was not accounted for. These breakthrough curves show that the retardation due to diffusion into and sorption within the matrix is different for breakthrough curves obtained in the same fracture. For fast paths the retardation is very small, but for slow paths the retardation is very important. For curves with short residence times, the retardation factor is 1.5 - 3. For those with long residence times this factor is as large as 50 - 500.

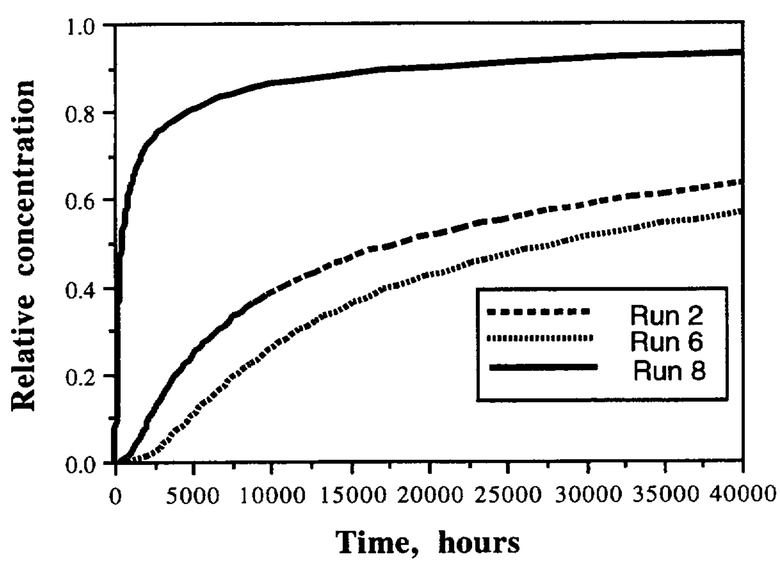


Figure 8. Breakthrough curves for some runs shown in Table 1, for a tracer that diffuses into the matrix and may sorb within the matrix.

7 SUMMARY OF DELIBERATIONS AND DISCUSSION

We have interpreted the overall aim of this experiment to gain a better confidence in models that will be used to predict the migration of radionuclides in the rock surrounding a repository. With this interpretation, those mechanisms that are significant for long residence times should be emphasized, and mechanisms which do not have a major influence can be neglected, unless they are important for interpreting the experiment.

Earlier field experiments and observations in fractured crystalline rocks show that fractures have strongly variable apertures. Water will seek out preferential flow paths, which may have strongly varying residence times and dispersion. The conventional advection dispersion model attempts to use average values for the aperture, and to describe the spread in residence times by what is called hydrodynamic dispersion. This effect is modeled as being caused by local velocity variations, which, when averaged, are assumed to behave phenomenologically in the same way as molecular diffusion. When using this type of model to describe the flow and transport in a fracture, the general idea is to determine some measure of the average aperture from the mean residence time of a tracer, and a dispersion coefficient from the spread in residence times.

Earlier attempts to do this have shown that when different paths in the same fracture are tested, the properties are found to differ considerably. It is by no means clear how such results should be used to make predictions of tracer transport in another path or over longer distances.

A further complication when using the conventional advection-dispersion-type model is that it gives no information on the so-called "flow-wetted surface." This is that part of the fracture surface that is in contact with the flowing water. Over this surface, the tracer and radionuclides will interact with the rock surface and diffuse into the matrix of the rock. The matrix diffusion and sorption onto the inner sites is the by far most important retardation mechanism for the radionuclides escaping from a repository.

To account for these effects, our concept of flow and transport in individual fractures is a variable aperture fracture with a porous matrix, in which solutes can migrate by diffusion. It is essentially a three-dimensional transport model, where the transport is by flow in two dimensions in the fracture plane. The transport in the rock matrix is by diffusion only. For tracers which do not have access to the rock matrix, either because the experimental time is short or because the molecules are so large that they cannot enter the pores, the model simplifies to a simple advection model in a two-dimensional strongly varying flow field.

The model needs only a few parameters. To describe the flow-rate distribution the local conductivity distribution must be known. For this form of the distribution (we use a log normal distribution), the mean value and the variance suffice to define the flow properties of the fracture.

Before considering any model-specific results, we wish to discuss some properties that are independent of the specific models considered in the MWTE. For a tracer that has no access to the porous matrix, the volume accessible to flow (the aperture distribution of the fracture) must be known in order to determine the residence time distribution, RTD, of the tracer. Interestingly enough, for tracers which have access to the porous matrix and for long residences times, the flow volume (or fracture aperture) has a negligible influence on the RTD. This is only determined by the flow-rate distribution, the "flow-wetted surface" and the diffusion and sorption properties of the rock matrix.

One of the inherent difficulties in the experiments is that the experimental time is so short that the so-called "conservative" tracers will not be influenced by matrix diffusion effects, and their RTD will thus only be influenced by variations in fracture aperture. The RTD of some slightly sorbing tracers that could conceivable be used will be influenced by both the water RTD and by matrix diffusion effects. It will not be possible to distinguish the two effects from tracer tests only. Nor will it be possible to estimate some measure of the "flow-wetted surface" with any confidence.

Theoretically, it could be possible to find a relation between the conductivity and the aperture. We assume in our calculations, knowing it may not be true in tight fractures of the kind we find in fractured crystalline rocks, that the cubic law is valid. This gives a simple relation between conductivity and aperture. With such a relation, the RTD found in tracer tests with non-interacting tracers could theoretically be used to confirm that the model exhibits the correct behaviour in both the observed flow rate (conductivity) distribution as well as the RTD. If such a relation cannot be found, the experimental RTD of non-interacting tracers cannot be used to help predict the migration of tracers that have access to the matrix.

If the main aim is to understand how solutes behave when the residence times are long, the usefulness of short term tracer tests is questionable.

So far, we conclude from considerations of the general mechanisms of tracer transport, which are model-independent and only based on what are general principles for solute transport, that it would be much more valuable to measure the conductivity distribution in more detail than to perform tests with "non-interacting" tracers.

A further general difficulty is that the conductivity of the fracture and other properties of interest for flow and transport are expected to vary by many orders of magnitude. A large number of measurements must be made to determine the proper form of the distribution and the parameters of the distribution. Hydraulic conductivity measurements are fast and cheap. They may be used in a straight-forward manner to determine the hydraulic conductivity distribution. Even distance short tracer tests take a long time and not many can be made. As indicated earlier, they are difficult to use for our ultimate purpose: to understand the migration during long times. There are, in addition, some difficulties that are specific to fractures with strongly varying apertures. Some of our simulations, as well as results from field experiments, show that the injection method may profoundly influence the RTD of the tracer. There are two main reasons for this. With low injection flow-rates, there is the distinct possibility that the injection point is in a low-flow region. It will take a very long time for the tracer to move out to the main flow paths, which are those we primarily wish to investigate. There are two ways to avoid this. One is to measure the local flow rate under existing flow conditions, and, if found to be low, to discard this point. The other way is to use a non-negligible injection flow-rate. This, however, causes other problems.

In section 4, the injection flow-rate was shown to have a large impact on the results of tracer tests. In some circumstances a large injection flow-rate can increase the residence time and dispersion of the tracers. This is because the injection modifies the pressure field around the injection point. If a large flow rate is used, the pressure around the injection hole will be higher and the tracers will seek new paths. This means that the tracers are spread over a larger zone around the injection point. Even small differences in injection flow-rates seem to be able to cause large differences in the RTD.

For sorbing tracers, the retardation may vary over a very wide interval. For the fastest channels this retardation may be very small. On the other hand, the slowest channels show a very large retardation. For example, in our simulations, if a value of 1.0 is used for $K_d \rho_p$, the fastest channels have a retardation factor of about 1.5-2.0, with almost simultaneous arrival with the conservative tracers. For the slowest channels, this retardation is substantial and the experiment would have a duration of years. These results are based on the results from simulations in one fracture. The variability between different fractures is large and the expected travel times in the fracture that will actually be used for the experiment may range from that of the non-interacting tracers to practically any length of time.

The present model concept, based on a variable aperture, has distinct advantages over the advection-dispersion and the channeling models that we have also considered. For the prediction of the migration of interacting tracers, one needs information on the hydraulic conductivity distribution over the fracture, in addition to the matrix diffusion and sorption properties. The latter entities must be known for every model if one wants to account for matrix diffusion effects. The magnitude of the flow-wetted surface will be obtained automatically when solving for the flow-rate distribution.

The advection-dispersion model needs data on some average flow rate in the fracture and on the dispersion. In addition, the magnitude of some average "flow-wetted surface" must be determined in some way. There are at present no accepted methods for doing this. The validity of the methods considered are easily challenged.

The channeling model with independent channels needs data on the flow-rate or conductivity distribution of the independent channels and their flow-wetted surface. Again, it is not clear how to obtain these.

8 RECOMMENDATIONS

During the experiment a very detailed measurement of the local hydraulic conductivity should be made at some fractures.

For the tracer tests several issues should be considered.

The injection flow-rate is an important parameter in tracer experiments. As discussed above, a very small or a very large injection flow-rate is not recommended. A large injection flow-rate in general increases the mean residence time and the dispersion. A small flow rate may significantly increase the travel time. For this reason the injection flow–rate should be, for example, larger than 0.1 %, and at the most a few percent of the withdrawal flow–rate.

The natural flow rate should be determined before using an injection hole. It should be discarded if it is low.

A number of tracers with different sorption properties must be used simultaneously in order to have a reasonable chance of recovering at least one in every flow path.

NOTATION

D_e	Effective diffusion coefficient	m^2/s
K_d	Volume sorption constant	m^3/kg
L	Length	m
P	Pressure	kg/ms^2
Pe	Peclet number	
Q	Water flow-rate	m^3/s
W	Channel width	m
r	Radial distance	m
R	Resistance	kg/m^4s
R_a	Surface retardation factor	
t_w	Water residence time	s
δ	Aperture	m
δ_o	Mean logarithm aperture	
λ	Correlation length	m
μ	Dynamic viscosity	kg/m s
ρ_p	Rock bulk density	kg/m^3
σ	Standard deviation in the log-normal distribution	
σ_t	Standard deviation in the breakthrough curve	s

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