

A method-of-characteristics concept for advective tracer transport in fracture networks

C. THORENZ, O. KOLDITZ & W. ZIELKE

Institut für Strömungsmechanik, Appelstr. 9A, D-30149 Hannover, Germany
e-mail: thorenz@hydromech.uni-hannover.de

Abstract The method-of-characteristics (MOC) is a well-known concept for the modelling of tracer transport, but it has not yet been adopted for transport in fracture networks. A method has been developed and implemented and this paper presents the concepts, applications and benchmark results.

INTRODUCTION

The simulation of tracer transport processes in fracture networks can be described either by volume averaged approaches (e.g. equivalent porous media) or by the direct modelling of discrete fractures and matrix blocks. Multiple numerical schemes are suitable for the modelling of transport processes, e.g. the finite-elements-method (FEM), the finite-volume-method (FVM), the method-of-characteristics (MOC) or particle tracking (PT).

In the past, the finite element simulator ROCKFLOW-3 (Kolditz *et al.*, 1998) was developed. The simulator is able to couple finite elements of different dimensions (1-D elements for favourite flow paths, 2-D elements for fractures, 3-D elements for the matrix) to reproduce the geometry of the underlying fractured rock system.

As the number of elements needed to represent the fracture system rises rapidly with the number of intersected fractures, a vast computational effort is necessary to perform a transport simulation, even if only the fractures and not the matrix are considered. The direct simulation of large fracture networks (i.e. hundreds of intersecting fractures) would be very useful to derive the parameters for volume averaged approaches. Furthermore any inverse modelling for parameter estimation requires an efficient numerical method, as the computational effort for inverse problems is even greater than for the direct problem.

As a solution for these objectives a Lagrangian approach is suitable. Earlier work (e.g. Geier *et al.*, 1995) presented the application of PT to fracture networks. In contrast to PT, the MOC requires the uniqueness of characteristics, which is not the case in fracture networks as mixing occurs at the intersections. This paper presents an extension to the MOC which enables the tracing of characteristics across intersections and therefore enhances the applicability of the MOC to fracture network simulations.

MATHEMATICAL MODEL

Governing equation

With the assumptions of non-deformable pore space, incompressible liquid and isothermal conditions, the governing equation for tracer transport is:

$$\frac{\partial c}{\partial t} = -v \cdot \text{grad}(c) + \text{div}(D \text{grad}(c)) + r \quad (1)$$

where c is the concentration of the tracer, t is time, v fluid speed, D is the combined Scheidegger–diffusion/dispersion tensor and r represents decay, sinks and sources in the system (Bear, 1972).

Operator splitting technique

$$\frac{\partial c}{\partial t} \approx \frac{c^{t+\Delta t} - c^t}{\Delta t} = \frac{c^{t+\Delta t} - c^{t^-}}{\Delta t} + \frac{c^{t^-} - c^t}{\Delta t} \quad (2)$$

This leads to the split form of the conservation equation (Hinkelmann, 1997):

$$\frac{c^{t+\Delta t} - c^{t^-}}{\Delta t} = v \cdot \text{grad}(c), \quad \frac{c^{t^-} - c^t}{\Delta t} = \text{div}(D \text{grad}(c)) + r \quad (3)$$

These equations can be solved separately by an adequate scheme, e.g. by a Lagrangian characteristics scheme for the advective part and an Eulerian finite element approach for the diffusive part (see Kolditz *et al.* (1998) for description). This has the advantage that the Courant criterion no longer has to be fulfilled so that a larger time step can be chosen for highly advective problems.

Method of characteristics (MOC)

The advective step of the split conservation equation:

$$\frac{c^{t+\Delta t} - c^{t^-}}{\Delta t} \approx \left(\frac{\partial c}{\partial t} \right)^- = -v \cdot \text{grad}(c) \quad (4)$$

which is equivalent to a zero total derivation:

$$\frac{dc}{dt} = 0 \quad (5)$$

i.e. the concentration remains conserved while following a characteristic at the fluid’s speed (e.g. Abbott, 1966). Therefore, the integration of velocity vectors over time gives a scheme to determine the new position of a fluid element at the new time level. At this position (the base point of the characteristic) the concentration is interpolated from the concentration of the surrounding nodes and is transferred back to the starting node (Fig. 1). This transfer is possible in both directions (forward or backward in time); in this implementation an upstream tracing has been chosen (i.e. characteristics are followed upstream or backward in time from a given node).

A particle tracker would compute the new position of one of the particles in a similar way, if only advection is regarded. The resulting concentration would be obtained by dividing the number of particles in a cell by the cell’s volume. A large

number of particles is necessary to achieve smooth approximations, while in a MOC scheme the number of characteristics to be followed is equal to the number of nodes.

Tracing of characteristics

Starting from a mesh node, the velocity vectors are followed from edge to edge in the mesh for each time step. During tracing, the given time step is used up while integrating the velocity vectors along the characteristic. Finally the tracing is stopped and the node values are interpolated from the surrounding nodes to the current position. This information is transferred back to the starting node (Fig. 1).

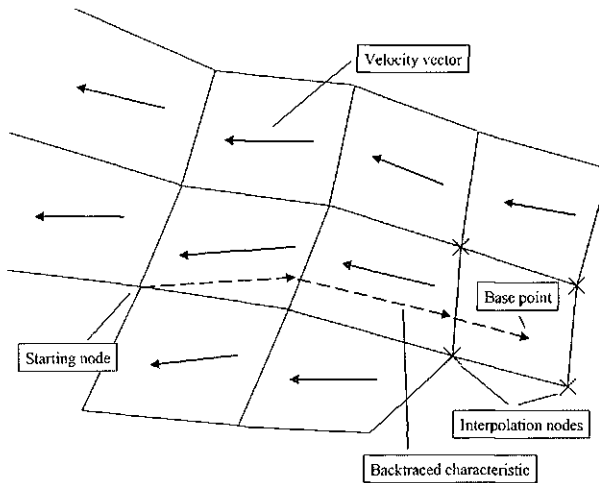


Fig. 1 Tracing of characteristics through the mesh.

Treatment of non-unique characteristics

The standard implementation of the MOC requires uniqueness of the characteristics followed. In fracture networks this uniqueness can not be guaranteed. The following method extends the capabilities to the tracing of characteristics over intersections.

Assuming total mixing at intersections the resulting concentration behind a single intersection (Fig. 2) can be computed as follows:

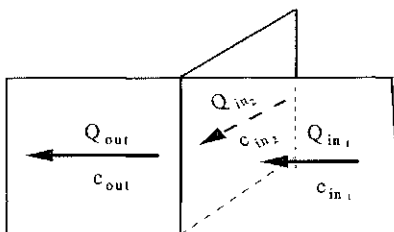


Fig. 2 Mixing at a single intersection.

$$c_{out} = \frac{\sum_{j=1}^{influxes} (Q_{in_j} c_{in_j})}{\sum_{j=2=1}^{influxes} Q_{in_j}} = \sum_{j=1}^{influxes} \left(\frac{Q_{in_j}}{\left(\sum_{j=2=1}^{influxes} Q_{in_j} \right)} c_{in_j} \right) = \sum_{j=1}^{influxes} (w_j c_{in_j}) \quad (6)$$

where c_{out} is the resulting concentration, Q_{in} are volumetric fluxes to the intersection, and c_{in} is the corresponding concentration of each flux. It is possible to introduce a local weighting factor w . This factor describes the influence of the upstream branches on the downstream branches and therefore on the starting node. A number of new characteristics (corresponding to the number of influxes) will be followed, each of them carries its individual weight w .

If a number of intersections i is crossed during the tracing, this concept has to be extended. At each intersection encountered, the weight will be distributed again by multiplying the previous weight of the characteristic with the new local weights. The sum of all weights in the system remains equal to one. The new node concentration c_{node} is gained by following a characteristic backwards in time across several intersections on its way. Thus the resulting concentration c_{node} is obtained as the sum of several results multiplied with the corresponding weight:

$$c_{node} = \sum_{j=1}^{base\ points} (w_j c_{in_j}) = \sum_{j=1}^{base\ points} \left(\left(\prod_{i=1}^{crossed\ intersections} w_i \right) c_{in_j} \right), \sum_{j=1}^{base\ points} w_j = 1 \quad (7)$$

Finally the resulting concentration is computed from the sum of the concentrations at a number of base points, each of them multiplied with the corresponding weight w_j . Therefore the main task is to determine the resulting weight w_j of a characteristics base point.

IMPLEMENTATION

The tracing along characteristics has been implemented in an object-oriented way. So called “agents” have been introduced, which are represented by a set of information (e.g. position, used travel time, weight) and methods (tracing and interpolation abilities). At each starting node a single agent is generated with a weight of one. Each agent travels along a characteristic until an intersection with more than one influx is reached. According to the number of influxes a set of new agents is generated, the old agent dies and passes weight and travel time to the new ones. The weight of each new agent is the result of the old agent’s weight multiplied by the new local weight.

Each agent travels until its time is used up (i.e. the end of the time step has been reached) and then reports its own weight and the interpolated concentration of the tracer back to the starting node, where both values are multiplied and summed up.

This scheme has been implemented recursively and is embedded into a loop over all nodes in the system. After all agents have reported back their weights and

concentrations, the total sum of weights per node should be equal to one. A small error can be encountered as characteristics with very little weight can optionally be neglected if the weight falls below an adjustable tolerance.

After the advective step the FEM core is started for the diffusive step. At this point decay and sources or sinks are integrated, too.

APPLICATION

For test applications fracture data from the Grimsel hard rock laboratory (4 fractures, geometry data provided by H. Shao, BGR), and Münchhagen site (11 fractures, geometry data provided by G. Kosakowski, GGA), have been used. These examples have been discretized with 3327 nodes (Grimsel) and 10 922 nodes (Münchhagen). The meshes were provided by H. Kasper.

Figure 3 shows tracer distributions of an injected tracer pulse in a system of four fractures. All methods give a similar distribution pattern, but the tracer peak is a little too dispersed in the operator-splitting scheme. Figure 4 shows the finite element mesh for a fracture system based on Münchhagen data. Again tracer transport has been computed with the different numerical methods.

Figure 5 allows the comparison of results for the peak breakthrough. The purely advective Lagrangian method computes very sharp peaks, whereas the FEM solution smooths the front. The operator splitting scheme shows results between the two, as is expected. Interestingly the Lagrangian scheme can reproduce one of the typical transport effects within fracture networks, the tailing effect. The network dispersion by macro-scale mixing processes starts to dominate over the neglected dispersion in the single fractures. For large fracture network systems this point of view might be sufficient for the problem description.

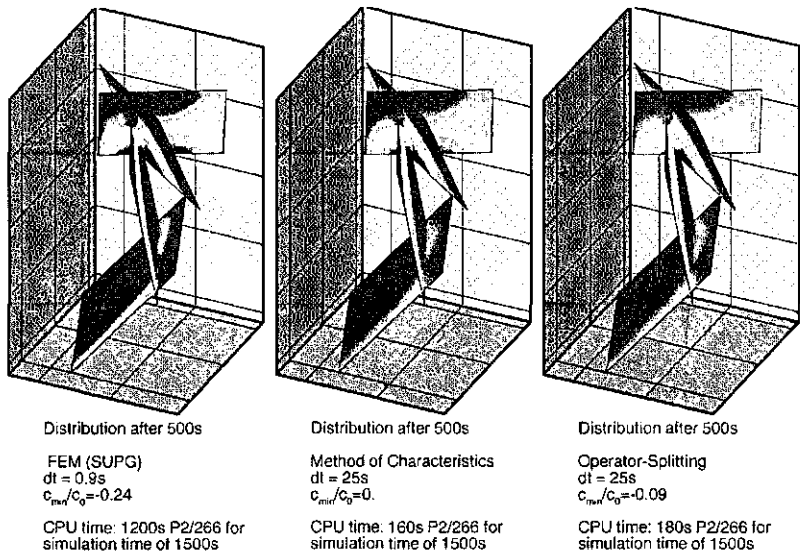


Fig. 3 Comparison of tracer breakthrough for a four fracture system (Grimsel) with different numerical methods.

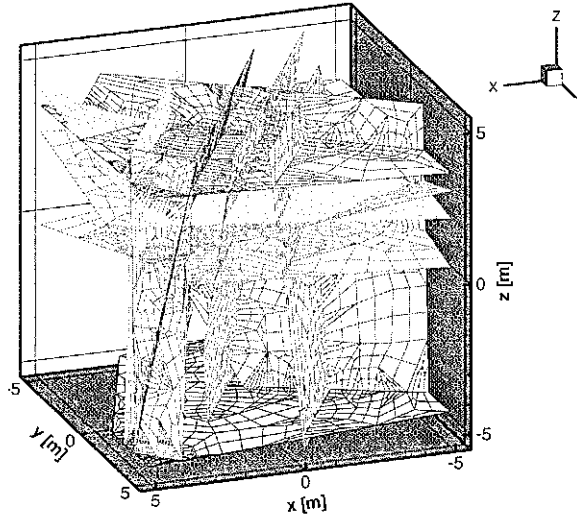


Fig. 4 Mesh for a system of eleven fractures (Münchehagen).

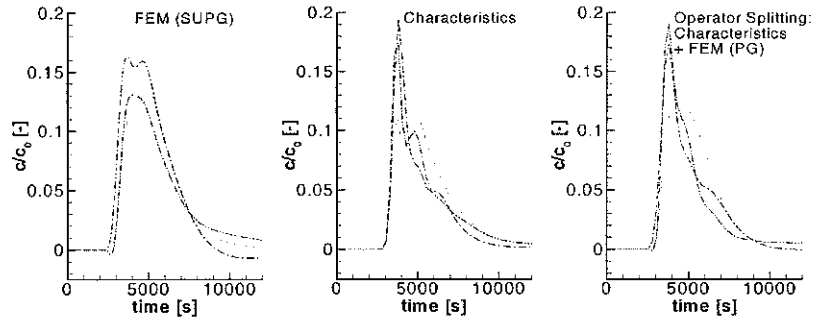


Fig. 5 Tracer breakthrough at three neighbouring outflow nodes for a system of fractures (Münchehagen) computed with different numerical methods.

The transport through the systems considered is highly advective ($Pe_{max} \approx 36$ for the first example, $Pe_{max} \approx 220$ for the second one). The Peclet numbers have been computed on the basis of local (single fracture) dispersivities, as the much larger total dispersivity results from macro-scale mixing in the network. For this kind of highly advective problem, an operator splitting scheme is very effective. Table 1 compares the necessary CPU times for the simulations mentioned above.

Table 1 Comparison of CPU time for different numerical methods.

	4 fractures, 3327 nodes, steady flow	4 fractures, 3327 nodes, unsteady flow	11 fractures, 10 922 nodes, steady flow
FEM (SUPG)	1065 s	5050 s	41312 s
Characteristics	38 s	481 s	577 s
Operator splitting FEM (PG) + characteristics	59 s	495 s	1018 s

CONCLUSIONS

- The extended MOC scheme presented is suitable for transport simulations in fracture networks. Macroscopic (network) mixing processes can be reproduced.
- By combination with the FEM, an operator splitting scheme is obtained which is able to simulate diffusion, dispersion, sorption and decay in an efficient way.
- For highly advective problems ($Pe \gg 1$) the MOC is very efficient
- For transport processes of tracers in large fracture networks the macroscopic mixing dominates over local diffusion and dispersion in single fractures, so that the very fast characteristics scheme is sufficient to describe the main processes.

REFERENCES

- Abbott, M. B. (1966) *An Introduction to the Method of Characteristics*. Elsevier, New York.
- Bear, J. (1972) *Dynamics of Fluids in Porous Media*. Elsevier, New York.
- Geier, J., Dershowitz, W., Wallmann, P. & Doe, T. (1995) Discrete fracture modeling of in situ hydrologic and tracer experiments in fractured and jointed rock masses. In: *Fractured and Jointed Rock Masses* (ed. by L. R. Myer & C. F. Tsang) (Proc. Lake Tahoe Conf., California, June 1992), 511–518. A. A. Balkema, Rotterdam, The Netherlands.
- Hinkelmann, R. (1997) Parallelisierung eines Lagrange-Euler-Verfahrens für Strömungs- und Stofftransportprozesse in Oberflächengewässern (Parallelization of a Lagrangian-Eulerian scheme for free surface flow and transport processes). PhD Thesis, Universität Hannover, Germany. *Report 51/1997 Inst. f. Strömungsmechanik, Universität Hannover, Germany*.
- Kolditz, O., Habbar, A., Kaiser, R., Schulze-Ruhfus, M. & Thorenz, C. (1998) *ROCKFLOW – Theory and Users Manual release 3.3*. Institut für Strömungsmechanik und Elektr. Rechnen im Bauwesen, Universität Hannover, Germany.