

MICROSCOPIC SIMULATIONS OF THE DISSOLUTION OF ROCK FRACTURES

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Summary

The results of numerical simulations of dissolution in fractured rocks are reported. The model is microscopic, with a detailed representation of the topography of the fracture. The velocity field in the fracture is assumed to be Stokes flow and is efficiently calculated with an implicit lattice-Boltzmann technique. The transport of dissolved species in the pore spaces is modelled by an innovative random walk algorithm that incorporates the chemical kinetics at the solid surfaces. The simulated morphological changes in a complex fracture are compared with laboratory experiments.

The processes leading to dissolution of a fractured rock by a reactive fluid depend on a subtle interplay between chemical reactions at mineral surfaces and fluid motion in the pores. The complex geometry of a typical fracture makes both numerical and theoretical calculations very demanding. Existing models of fracture dissolution are rarely constructed on a microscopic (pore-scale) level. Instead, various approximations are usually resorted to in order to make the analysis more tractable. For example, instead of computing a three-dimensional velocity field by solving the Navier-Stokes equations, the Reynolds (or lubrication) approximation is used [1, 2, 3], so that the volumetric flow rate is proportional to the cube of the local aperture. It has been shown [4, 5, 6] that the Reynolds equation may significantly overestimate the flow, especially for fractures of high roughness and small apertures. The complicated topography of the fracture is also the reason why the transport of the dissolved material from the walls into the bulk of the fluid is usually accounted for in a simplified way, with the effects of convection assumed to be adequately expressed by a Sherwood number for transport in ducts [1, 2, 7]. However fracture erosion is a complex process involving nonlinear feedback mechanisms. Thus a relatively small change of topography may result in a large variation in permeability, leading to further changes in erosion. These instabilities make it hard to estimate or control the effects of approximations, so there is a need for precise numerical algorithms that allow for a full microscopic simulation of the fracture dissolution process.

In our implementation of the erosion algorithm, the velocity field in the fracture is calculated using the lattice-Boltzmann method with "continuous bounce-back" rules applied at the solid-fluid boundaries [8]. These rules allow information about the solid surface on length scales less than a grid spacing to be resolved. Therefore, it is possible to adequately resolve the flow field with one-half to one-quarter the linear resolution of the traditional lattice Boltzmann method. Furthermore the steady-state solution is determined directly, using conjugate gradients [9], and is at least an order of magnitude faster than time stepping. These improvements allow us to calculate velocity fields in fractures with a characteristic size of several centimeters.

Solute transport in the fracture is modelled by a random walk method, which takes explicit account of the chemical reactions at the pore surfaces. The fracture surface is divided into pixels, typically 200-500 per dimension, and the height of each pixel is eroded in response to contacts by tracer particles. The major drawback of the classical random walk method [10] is that in order to calculate the dissolution fluxes a very large number of particles must be tracked simultaneously so that the concentration in the fluid near the pore surface can be determined accurately. However, there is a considerable simplification in the case of linear dissolution kinetics, where the erosion flux through the interface, J , is given by

$$J = r(c_s - c_0); \quad (1)$$

here c_0 denotes the solute concentration at the interface, c_s is the saturation concentration, and r the rate constant. In this case it is possible to derive a single-particle stochastic propagator which satisfies the boundary condition 1. Using this propagator, one can find the dissolution fluxes in the fracture by tracking a single particle at a time. Such a scheme is several orders of magnitude more efficient computationally and can be used to calculate the concentration profiles in very large fractures. The evolution of the fracture morphology is then determined by removing material from the fracture walls in proportion to the local dissolution flux calculated in the random walk step. The time evolution of the velocity field and local aperture field in the fracture are determined by iterating this procedure, removing small amounts of material at each step.

We have studied the evolution of fracture topography in several different geometries, including artificial fractures created numerically and topographies for which experimental data also exists [11]. The dissolution simulations were performed over a wide range of Pelet and Dämkohler numbers. The Pelet number measures the relative magnitude of convective and diffusive transport of the solute, $Pe = v \langle h \rangle / D$, where v is a characteristic fluid velocity, $\langle h \rangle$ is the mean aperture and D is the solute diffusion coefficient. The Dämkohler number, $Da = k/v$, relates the surface reaction rate to convective transport. In a number of experimental and numerical studies [11, 12] it has been established that the dissolution patterns depend strongly on the values of Pe and Da . These results have been confirmed in the present study. For small values of Pelet number and large values of Dämkohler number the fluid saturates completely at or near the injection face. As a result, after the initial fast dissolution of the rock material at the fluid inlet, the reaction front propagates extremely slowly, as there is almost no unsaturated fluid penetrating inside the fracture. On the other hand, when the flow rate is large and the reaction rate relatively slow, the unsaturated fluid penetrates deep inside the fracture and

the dissolution tends to be uniform throughout the sample. The most interesting phenomena are observed for moderate values of Da and Pe . Here, the nonlinear feedback mechanism mentioned above begins to play an important role. A perturbation in the reaction rate at the advancing dissolution front changes the local permeability which in turn affects solute transport and the dissolution rate. As a result, the front becomes unstable and pronounced channels are formed in which most of the flow is focused while most of the pore space is eventually bypassed. As an example, Fig. 1 present snapshots of the fracture flow field evolution for $Pe = 10$ and $Da = 0.1$. The successive plots show the vertically (fracture normal) averaged momentum flow before dissolution and after 8, 16, 24, 32 and 40 dissolution cycles respectively. In each step, the total volume of material dissolved was equivalent to a layer of about 1% of the mean aperture. The initial fracture geometry was prepared numerically, with a mean aperture equal to 1% of the length. Under these conditions the initially uniform flow is rapidly replaced by a few pronounced dissolution channels. As the dissolution proceeds, the channels compete for the flow and, the growth of the shorter channels eventually ceases. This is in the agreement with the results of Hoefner and Fogler [13] who claimed that the difference in the lengths between two channels is unlikely to exceed the distance between them. After about 30 iterations most of the flow is focused in the single main channel, which after about 40 iterations connects to the outflow end of the fracture. This breakthrough is accompanied by a huge increase in fracture permeability.

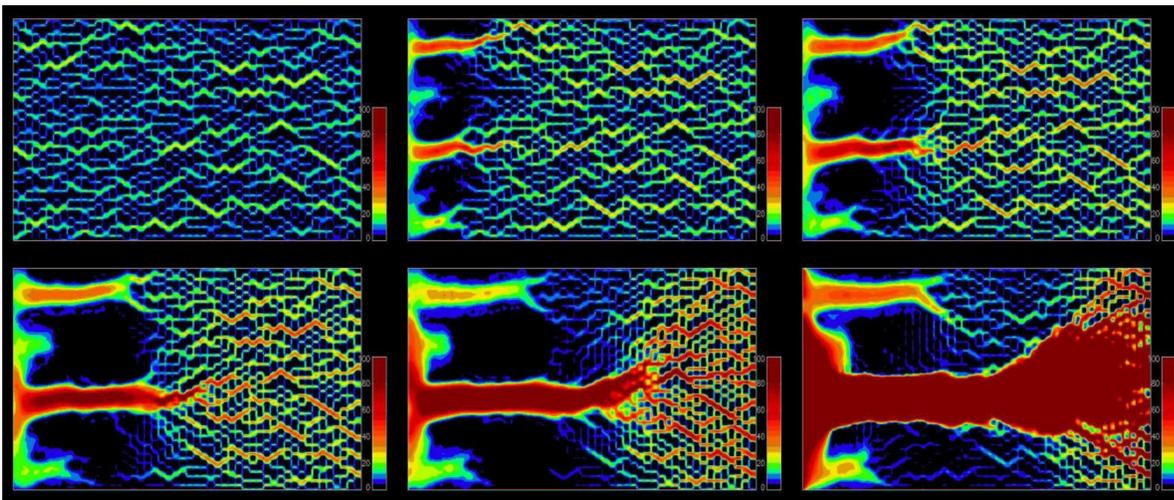


Figure 1. The vertically (fracture normal) averaged momentum flow before dissolution and after 8,16,24,32 and 40 iterations respectively. The colors indicate regions of low (blue), medium (green), and high (red) flow rates. The scale is the same in each picture.

In conclusion, we have developed a fully microscopic numerical method to simulate the dissolution of rock fractures on experimentally relevant length scales. Dissolution morphologies similar to those seen experimentally have been observed. The method may be used not only to analyze the dissolution patterns in various fracture geometries, but also to test the validity of the approximations typically used in fracture erosion models.

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