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Deposition and/or dissolution in Porous Media

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The major objective of this project which is part of the European Training Network IMVUL is to devise and develop a new generation of basic numerical tools able to analyze the state and evolution of mineral microbe systems which may induce permeability reduction and clogging of aquifers. These tools will be validated and compared to experimental results in collaboration with the University of Edinburgh.

Bekri et al (1997) developed a first generation of codes in order to analyze the evolution of porous media due to dissolution or dissolution of flowing species. Among the main features of this model, one can mention that the porous medium was discretized by cubic voxels, that the chemical reaction was first-order and that the analysis was restricted to a quasi steady evolution, i.e. to limited values of the Dahmkohler number.

Four types of improvements are implemented.

First, the solid-liquid interface is tracked by means of the Level set method (LSM). In this method, the real surface is defined by a distance function based on the usual fixed Cartesian grid. The interface is represented by a polygonal smooth surface at the zero level of this distance function. The advantages of the level set method include (a) we are able to compute geometric quantities easily, (b) the result is accurate and the codes are faster than the ones based on a cubic space discretization and (c) it handles topology propagation effectively. The most challenging difficulty is that this method requires a special treatment of the boundary conditions at the level set surface.

Second, the transport phenomena on the pore scale are governed by the Stokes equation of motion and by the convection-diffusion equation supplemented by a condition on the deposition/dissolution flux at the walls. This coupled problem was not often investigated, especially for random media represented by the Level Set method. The most important improvement is that the boundary conditions are written at the level set surface and not at the discretized surface by voxels. Furthermore, the flux to the interface is precisely computed by using the unit vector which is normal to the smooth surface.

Third, the chemical reaction is extended to biofilms where the reaction at the fluid-solid interface obeys the Michaelis-Menten kinetics (hyperbolic form). This reaction which is very common in biology and medicine has an additional parameter of half-saturated concentration.

Fourth, direct time simulations or quasi steady simulations can be performed. For the slow reaction rate, for the sake of simplicity, the analytical and numerical solution usually assumes that the system is quasi-steady a long time after the beginning of the injection. However, for faster reaction rates, this assumption could cause a considerable error. The differences between the results of these two simulations will be estimated.

After a brief presentation of these improvements, tests and first applications of the code which is now working, are given. The effect of the discretization method and of the numerical resolution of the equations, the accuracy and the efficiency are further documented.

Some comparisons with analytical solutions in a simple configuration are first performed to validate the code. Three-dimensional reconstructed porous media based on thresholded correlated Gaussian fields are represented by the Level Set method. The influence of the reaction rate, the transport conditions and the initial geometry are then systematically explored in detail in three dimensions.

S. Békri, J.-F. Thovert, P.M. Adler, Engineering Geology, 48, 283, 1997