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Pore network and pore scale modelings of reactive transport in porous media

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The study of the evolution of a porous medium where a reactive fluid flows, is conditioned by the accurate determination of macroscopic parameters governing the solute displacement, namely the solute velocity, dispersion and mean reaction rate. Of course, a possible application of such studies is CO_2 sequestration.
This presentation proposes to approach the determination of these parameters by two different ways and to compare them; both are on the pore scale.
In the first one called PNM (for pore-network model), a pore-network is extracted from micro tomography images of a real porous medium. This network is composed of spherical pores joined by circular tubes; it is used to calculate transport macroscopic parameters and porosity-permeability evolution during the reactive transport flow as functions of dimensionless numbers representing the reaction and flow rate regimes. The flow calculations are made with Kirchhoff laws. The transport calculations are performed in the asymptotic regime where the solute concentration undergoes an exponential evolution with time.
In the second approach (called pore scale), the pore-network model is used as a three dimensional medium which is discretized by the Level Set Method. The Stokes equations are solved in order to determine the local flow field and the corresponding permeability. In very much the same way, the solute concentration is obtained by solving the local convection-diffusion equation in the three dimensional pore-network model; in order to reduce numerical dispersion, a Flux Limiting Scheme is used to discretize the equations.
Then, the results obtained by the two approaches are compared. Permeability is obtained with a good accuracy by both techniques. The concentration fields and the overall reaction rate are compared for a small and a large pore network. The concentration fields are remarkably similar for the two approaches as well as the overall reaction rates. Still more remarkable is the common prediction of the surprising evolutions of these fields when the Péclet number varies.
One of the main provisory conclusions of this work is that PNM can address much larger samples than pore scale models and can therefore be a tool of choice to study transforming porous media.