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Modeling of Flow, Transport and Controlled Sedimentation Phenomena during Mixing of Salt Solutions in Complex Porous Formations

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The deposition of salts in porous media is a major engineering phenomenon encountered in a plethora of industrial and environmental applications where in some cases is desirable and in other not (oil production, geothermal systems, soil stabilization etc). Systematic approach of these problems requires knowledge of the key mechanisms of precipitating salts within the porous structures, in order to develop new methods to control the process.

In this work, the development and the solution of spatiotemporally variable mass balances during salt solution mixing along specific pores were performed. Both analytical models and finite differences CFD models were applied for the study of flow and transport with simultaneous homogeneous and heterogeneous nucleation (by crystal growth on the surface of the pores) in simple geometries, while unstructured finite elements and meshless methods were developed and implemented for spatial discretization, reconstruction, and solution of transport equations and homogeneous / heterogeneous reactions in more complex geometries.

At initial stages of this work, critical problem parameters were identified, such as the characteristics of the porosity, the number of dissolved components, etc. The parameters were then used for solving problems which correspond to available experimental data. For each combination of ions and materials, specific data and process characteristics were included: (a) crystal kinetics (nucleation, growth rates or reaction surface rates of crystals, critical suspension concentrations), (b) physico-chemical properties (bulk density, dimensions of generated crystals, ion diffusion coefficients in the solution), (c) operating parameters (macroscopic velocity, flow, or pressure gradient of the solution, ion concentration) (d) microfluidic data (geometry, flow area), (e) porosity data in Darcy description (initial porosity, specific surface area, tortuosity).

During the modeling of flow and transport in three-dimensional pore network, the dependence of the mass balance in all major directions is taken into account, either as a three-dimensional network of pores with specific geometry (cylinders, sinusoidal cells), or as a homogeneous random medium (Darcy description). The distribution of the crystals along the porous medium was calculated in the case of selective crystallization on the walls, which is the predominant effect to date in the experiments. The crystals distribution was also examined in the case where crystallization was carried out in the bulk solution. Salts sedimentation experiments were simulated both in an unsaturated porous medium and in a medium saturated with an oil phase. A comparison of the simulation results with corresponding experimental results was performed in order to design improved selective sedimentation of salts systems in porous formations.

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