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Barite precipitation in porous media: from tomography experiment to simulations

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Understanding reactions in porous materials impacts a wide range of applications including CO2 sequestration, hydraulic fracturing, design of energy storage systems, and supported catalysts. Particularly, the fundamental problem of crystal formation in porous materials raises two important questions: how is the crystallization process affected by the confined space [1], and how can we control the crystal growth in porous matrices? The barite (BaSO4), one of the minerals which often accompanies hydraulic fracturing during oil and gas extraction, also considered as a potential material for contaminant confinement due to the ability to incorporate, for example, radium and strontium ions into the crystal lattice.
Previous studies of barite crystal growth on glass surfaces [2,3] have shown that the growth rates of individual crystal faces respond nonproportionally to solutions at different saturation index and ionic strength. Also effect of surface hydrophobicity on heterogeneous nucleation of barite has been studied. We also carried out first in situ experiments of barite precipitation in pores [4] where correlations between pore size, fluid velocity, and crystal nucleation rate were observed.
Our recent X-Ray computed tomography (XCT) experiments on barite precipitation in porous systems formed by glass beads packed into a capillary, have shown that the morphology of the precipitate depends on the flow rate and presence of impurities (strontium cations). In this case strontium affects not only a crystal growth rate, but also the morphology of the precipitate. We have applied segmentation to XCT data to determine the interface between solid and fluid, and then used an OpenFOAM machinery to generate a body fitted mesh to use it in finite volume approach for simulation of the flow and reaction within the initial porous space and porous space with precipitate.

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References

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