

Pore scale experimental and computational analysis of reactive transport in a natural limestone

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Reactive transport processes in porous media have a significant impact on many subsurface energy activities including in-situ, ex-situ carbon sequestration, long-term performance of enhanced geothermal systems, geologic hydrogen storage, unconventional resources recovery among others. Over the past two decades, our understanding of pore-scale reactive transport processes has been dramatically improved through both experimental and computational studies (e.g., Yoon et al., 2015; 2019). In this work fluidic systems made of a natural limestone are used to evaluate reactive transport processes including dissolution and precipitation. A wide channel system on the surface of the limestone is used to evaluate the impact of different influent solution chemistries over pH and ion species on chemical reaction rates, reaction feedback on hydrodynamics, and their coupling process. The reactive flat surface is characterized for surface roughness and elemental/mineralogical mapping is performed after experimental works. During reactive transport experiments reactive surfaces are monitored using optical and confocal microscopy as well as analysis of effluent solution. A hybrid lattice Boltzmann-finite volume (LB-FV) approach for reactive transport including dissolution and precipitation processes is used to analyze experimental observations. To improve computation efficiency dramatically a GPU-based LB simulation will be employed to account for hydrodynamics and machine learning-based model (e.g., convolutional/artificial neural networks) for chemical reaction speciation will be developed and applied for reactive transport processes. In this presentation we will highlight how experimental observations including dissolution and precipitation through imaging and solution chemistry can be utilized to validate pore scale modeling to improve our understanding of calcium carbonate precipitation and dissolution processes in the natural limestone. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

References

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