Pore-Scale and Continuum Simulation of Microfluidics Experiments on Reactive Transport and Multiphase Flow conducted at EMSL

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Advances in microfabrication and imaging technology have enabled direct observation of coupled flow and reaction process at the pore scale. A state-of-art user facility was developed at EMSL to enable direct application of these advances to the study of pore scale processes in groundwater and deep subsurface reservoirs. Similar advances in computing power and numerical methods allow for direct numerical simulation of pore-scale processes from first-principles without any adjustable parameters. Investigators at the University of Illinois have been collaborating with EMSL scientists to conduct pore-scale experiments and simulations to investigate a variety of processes, including mixing-controlled aqueous reactions, mixing-controlled precipitation, and multi-phase flow. These processes are important to understand for many science and engineering questions, including contaminant fate and transport, biogeochemical dynamics in the root zone, and geological sequestration of carbon dioxide. By combining pore-scale simulation and experiments we have studied the impact of pore geometry and flow rate on mixing, how mixing and solution composition affects precipitate mineralogy, stability, and pore blocking, and the impact of flow rate and pore geometry on two-phase saturation and interfacial area. Numerical modeling allows testing of hypotheses about fundamental reaction mechanisms provides a tool for upscaling.