Integrated Experimentation and Hybrid Modeling for Prediction and Control of Multi-Phase Flow and Reaction in CO2 Injection and Storage

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The prediction and control of multiphase flow and reaction in geologic media is one of the great challenges in the Earth and Energy Sciences. This challenge has come into even greater focus with the recognition that the environment cannot sustain the CO_2 released from oil, gas, and coal combustion. These carbon-based fuels form the backbone of the world economy and have enabled nearly all of the technological innovations of the past 100 years. As developing countries with large populations strive to attain higher standards of living, their emphasis will be on the utilization of even more inexpensive and abundant fossil fuel (e.g., China is currently completing construction of more than one coal plant *per week*). A promising approach for avoiding this impending environmental crisis is the geologic sequestration of CO_2 in depleted oil reservoirs and deep saline aquifers.

We have identified five scientific challenges organized around the theme of mobility of CO_2 and that address the fundamental behavior of multiphase flow and reaction in porous media: 1) *Flow Patterns and the Dissolution of CO_2*; 2) *Capillary Trapping of CO_2*; 3) *Chemical Reactions of CO_2 with Rock*; 4) *Gravitational Mixing of CO_2-Saturated Brine*; and 5) *Development of a Hybrid Numerical Scheme to Couple Pore- and Continuum-Scale Processes*. We attack these problems with a philosophy that understanding CO_2 behavior begins with pore-scale, interfacial phenomena and involves determining how macroscopic properties emerge from the collective behavior of the pore-scale systems. Our team brings novel experimental methods that will allow for the *first time* direct observation of high-pressure, supercritical CO_2 interactions with pore-scale systems using microfluidics and x-ray micro-computed tomography. We will repeat these experiments at the laboratory-scale making direct observations with neutron tomography and we use CO_2-analog systems to explore large-scale phenomena in 2-D flow tanks (Hele-Shaw cells) and in 3-D flow tanks (“sand boxes”) using magnetic resonance imaging (MRI). We will simulate the pore- and laboratory-scale experiments at unprecedented detail using a state-of-the-art multiphase, multicomponent lattice Boltzmann (LB) model and a massively parallel, multiphase continuum flow and reaction code. And finally, we bring these scales together to make quantitative predictions of CO_2 mobility using a novel hybrid modeling scheme in which LB pore-scale calculations at reaction fronts are coupled to a continuum model of system-wide behavior.