

HYBRID PORE-SCALE SIMULATIONS OF CALCITE PRECIPITATION IN A CO₂ RICH ENVIRONMENT

Alexandre M. Tartakovsky* and Sebastien Kerisit†

* Pacific Northwest National Laboratory, Richland, WA 99352, US
e-mail: Alexandre.Tartakovsky@pnl.gov

† Pacific Northwest National Laboratory, Richland, WA 99352, US
e-mail: Sebastien.Kerisit@pnl.gov

Summary. A hybrid model was developed for calcite precipitation in a CO₂ rich environment. A Kinetic Monte Carlo model coupled with a solution of the classical diffusion equation was used to calculate the rate of a calcite precipitation-dissolution reaction for solutions with different pH and temperature. A Smoothed Particle Hydrodynamics method was used to simulate a pore-scale injection, entrapment and dissolution of a supercritical (sc) CO₂ as well as the calcite precipitation. Different mechanisms of sc CO₂ entrapment were investigated including dissolution of a sc CO₂ plume and the upward mobility of a sc CO₂. The effect of Raleigh-Taylor instability on the rate of CO₂ dissolution was also studied. KMC and pore-scale simulations were used to calculate the effective rate of sc CO₂ dissolution and the effective rate of calcite precipitation/dissolution in the CO₂ rich environment.