

Numerical Simulation of Kinetic Interface Sensitive Tracer in Experiment with COMSOL Multiphysics® Software

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Abstract

The kinetic interface-sensitive tracers (KIS tracers) developed by Schaffer et al. is used to give a partial picture of the spreading, mixing and plume migration of supercritical carbon dioxide (scCO₂) in the deep saline aquifer by estimating the interfacial areas between scCO₂ and brine during the injection of scCO₂. To get a better understand of the KIS tracers development, it is necessary to build a numerical transport model, which can express the tracer reaction and transport process in the two-phase flow system.

Based on the experimental breakthrough data, a novel approach for modeling KIS tracers with respect to specific interfacial area was developed in COMSOL Multiphysics® software. The two-phase flow system was built up by applying the pressure-saturation equations using the Coefficient Form PDE interface. And the solute transport process was simulated in the Transport of Diluted Species interface, based on the mass balance equation of each component in each phase. By introducing the interface mass transfer rate, which linearly depends on the kinetic reaction rate, specific interfacial area and fractional occupancy of the adsorption sites the specific mass flux of the reaction products into the water phase can be expressed. This novel model overcame the drawbacks of the current standard multiphase multi-component models which ignored the kinetic of mass transfer over the interface.

The numerical model indicate an abrupt interface separating non-wetting phase and wetting phase, which means a narrow transition zone between these two fluids. The breakthrough behavior of KIS tracer reaction product was expressed as a two-stage development: the early linear concentration development stage and the constant concentration stage. By analyzing the sensitivity of the product concentration, a better hypothesis on the reliable value of the kinetic reaction rate for further experiments and KIS tracer design was found. Furthermore, different pc-Sw-awn equations were tested to estimate specific interfacial area between n-octane and water.