

The Petroleum Engineering Department Presents

Pore-Scale Reactive Transport Modeling of Subsurface Water-Rock Interactions

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Abstract

Understanding of reactive transport is of fundamental importance to various applications in subsurface systems of energy and resources. Such subsurface formations as natural shales have rich compositions with carbonate, clay, sulfide, and quartz. In such systems, mineral-fluid interactions have critical impacts on the fluid transport, as subsequently resulting in the porosity-permeability alteration, pore geometry alteration, and flow pathways evolution. In this regard, the present dissertation establishes the pore-scale reactive transport models to investigate the impacts of mineral-fluid interactions on fluid transport. The present dissertation mainly focuses on three mineral-fluid interactions: carbonate dissolution, clay swelling, and iron precipitation from sulfide (pyrite). Here, we take quartz as a non-reactive mineral. These three mineral-fluid interactions are investigated through the following specific application problems: calcite dissolution by hydrochloric acid (to investigate the carbonate dissolution), CO₂-enriched brine injection (to investigate the carbonate dissolution and clay swelling), and hydraulic fracturing fluid injection into shale (to investigate the iron precipitation).

In the first application problem, the developed pore-scale reactive transport model is applied to the calcite dissolution by hydrochloride acid on the ideal grain models, digital rock images such as Niobrara formation, and fractures with surface roughness. The effects of Damköhler number (Da_{II}), Péclet number (Pe), the heterogeneity of the pore structure, and the mineralogy on the dissolution pattern, porosity-permeability relationship, and dissolution rate are investigated. The different dissolution and transport patterns are categorized with respect to the Da_{II} and the Pe . We also find that the dissolution of pore was significantly influenced by the Da_{II}/Pe ratio. Da_{II}/Pe ratio need to be larger than 1 to guarantee effective acidizing. For highly heterogeneous grain distributions, larger Da_{II}/Pe ratio gave rise to the thorough consumption of the calcite. If the grains are mainly distributed around the injection well, smaller Pe can be recommended considering the economic feasibility. We notice that the porosity-permeability relationships are significantly depending on the surface roughness factor of the fracture.

In the second application problem, the reactive transport model is coupled with the momentum conservation equation for plastic solid to describe the clay swelling during the injection of CO₂-enriched brine into the systems with mixed minerals of calcite, clay, and quartz. The porosity-permeability relationships with pure calcite, calcite-quartz, and clay-calcite of fracture-matrix systems are investigated. In addition, the impacts of fracture length, density, and connectivity on the fluid transport, porosity-permeability relationship, and evolution of pathways are studied. When the system contains clay, the permeability increase has been slowed with respect to the porosity increase induced by calcite dissolution. In this regard, clay can be used to increase the sealing capacity for CO₂ storage.

In the third application problem of hydraulic fracturing fluid injection into shale, we first conduct the experiments with the pyrite sample to calibrate the reaction rate constant for the pyrite oxidation. This reaction rate constant is utilized to establish the numerical method to track the iron precipitation on the pyrite surface by applying the Level-set method. The precipitation pattern on the digital rock image is investigated under different Damköhler numbers by a conceptual model. Under the larger Da_{II} , the precipitation has longer dendritic shape.

The quantified pore-scale parameters obtained from this study are expected to improve current Darcy-scale models to accurately predict the long-term fate for the subsurface water-rock interactions.