Direct pore-scale numerical simulation of precipitation and dissolution

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Mineral precipitation and dissolution driven by field applications such as carbon sequestration or remediation strategies can modify the geometry and structure of porous media in relatively short time scales. In this context, feedback processes between geochemical reactions and flow that take place at the pore scale affect continuum scale parameters such as permeability or reaction rates. Beyond the insights gained by innovative experimental and imaging techniques such as x-ray computed micro-tomography, modeling provides a unique tool to mechanistically understand and quantify these feedback processes at the pore scale and inform continuum scale models. In this work, we develop strategies to perform efficient direct numerical simulation of flow and reactive transport on idealized and complex pore scale geometries building on existing platforms. We apply these approaches to a range of pore geometries from single pores to 1-cm-long columns to calculate average reactions rates and porosity-permeability evolution and illustrate model capabilities and limitations.

Simulations show that dissolution and precipitation reactions affect the pore space nonuniformly. As a result, a simple porosity-permeability correlation may be insufficient to describe the complexity of the reaction-induced pore space evolution. The relative magnitude of the reaction rate constants affects the evolution of the permeability-porosity relationship. In dissolution simulations, fast reactions result in localized effects and further evolution of permeability is relatively unaffected by subsequent porosity increase. In contrast, slow reactions cause a less localized dissolution, with the result that the permeability increase is consistent with the porosity increment. Simulations show that in columns with the same average parameters, including column porosity, reactive surface area, and flow rate, different pore structures with different flow patterns can result in different average reactions rates.

Sequential coupling between transport and geochemical reactions allowed us to use an efficient and flexible computational fluid dynamics platform that implements higher-order algorithms, while implicit coupling shows promising results for efficient simulation of pore geometry evolution. We discuss further model development for interpretation of experimental results.

Genetic relation between Skarn ore deposits and magmatic activity in the Ahar region, Western Albuorz, northwest of Iran: Evidence for metasomatism and copper mineralization

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Numerous skarn deposits formed in the contact between the Upper Cretaceous impure carbonate rocks and Oligocene–Miocene Magmatic rocks in the Ahar region. The aim of this study is to understand how magmatic activity led to the copper skarn mineralization in this region. The history of skarn formation starts with the emplacement and upwelling pluton body, followed by the assimilation of limestone by the magma. The skarnification process occurred mainly in two stages: the first stage is starting with prograde metasomatism and anhydrous minerals, this stage followed by four stages of retrograde skarn deposit. In addition to Fe, Si and Mg, substantial amounts of Cu, along with volatile components such as H_2S and CO_2 were added to the skarn system. Consequently considerable amounts of hydrous calc-silicates, sulfides, oxides and carbonates replaced the anhydrous calc-silicates and the chemistry of the host granodiorites, Mineralogical and chemical characteristic indicate that an island arc or Subduction-related origin of Fe-Cu skarn deposit.