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A multiscale model for coupled chemical reaction and deformation of porous rocks

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Coupled hydro-mechano-chemical (HMC) modeling is a topic of active ongoing research in various branches of Earth sciences and subsurface engineering. In engineering applications, HMC modeling is used to assess the feasibility of permanent CO₂ storage in mafic and ultramafic rocks. The deformation and stresses building during the reaction is believed to induce fracturing, increase permeability and thus promote extensive reactions between CO₂ and host rock. CCS in depleted reservoirs faces challenges related to possible CO₂ leakage through old plugged and abandoned wells. When CO₂ reaches the well, old cement compositions react with cement, compromising well integrity due to chemical degradation. In geology, coupled reactions and deformation are involved in melt extraction and migration, influencing the dynamics of volcanic systems and the evolution of subduction zones.

A large focus of previous studies was whether or not it is possible to achieve 100% of the reaction. Common reactive transport models predict that the reaction product will clog the pores, which will stop the fluid flow and thus further reactions. However, recent developments suggest that reaction progress depends on the assumed reaction kinetics and the constitutive models used in coupled models. Models that account for solid volume change as in mineral replacement reactions have a much higher potential for preserving porosity than the common dissolution-precipitation model, thus predicting the complete reaction. It is often assumed that reaction processes are transport-dominated, i.e., that all dissolved material is carried away by pore fluid. Then it precipitates on the available pore space leading to clogging and permeability reduction. However, recent observations suggest that while some reactions might be associated with dissolution and precipitation at the nano-scale, aqueous species transport is limited, and reaction products do not precipitate in the pores but rather stay attached to the primary mineral. Thus, the overall effect is the same as in mineral replacement reactions.

Using a combination of effective media theory and irreversible thermodynamics approaches, we propose a new model for reaction-driven mineral expansion, which preserves porosity and limits unrealistically high build-up of the force of crystallization by allowing inelastic failure processes at the pore scale. To fully account for the coupling between reaction, deformation, and fluid flow, we derive macroscopic poroviscoelastic stress-strain constitutive laws that account for chemical alteration and viscoelastic deformation of porous rocks. These constitutive equations are further

used with macroscopic conservation laws to illustrate the mutual impact of reactive transport and mechanical deformation on simple 1D examples of wellbore stability and fluid transport.