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Mineral nucleation and its role in governing permeability/diffusivity modification

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Despite the fact that reactive transport modeling has been established as an indispensable tool in earth and environmental studies, it is striking how little progress has been made in implementing mineral-fluid rate laws that capture the entire set of dynamic processes from nucleation, to crystal growth, to mineral aging and transformation via the Ostwald Step Rule. Arguably the first such model was developed and implemented in a reactive transport (RT) framework by Steefel and Van Cappellen in 1990, who based their approach at the time on the calculation of a crystal size distribution (CSD) that transformed as a function of time and environmental conditions. An approach is explored in this presentation wherein discrete mineral "pools" are included in the RT framework that may represent either distinct mineral phases (as in the classical Ostwald Step Rule), or may be separate pools of the same mineral with different properties (e.g., specific surface area, intrinsic reactivity, or solubility). Transformation rates from one mineral pool to another are governed by semi-empirical rate constants based on the thermodynamic driving force and the mass or surface area of the reacting phase. Nucleation is treated within the continuum framework with largely classical exponential rate laws that depend on the supersaturation and interfacial free energy. The simulations demonstrate that nucleation may exert an important control on the subsequent permeability and/or diffusivity modification of the subsurface material, since heterogeneous nucleation will determine where the secondary mineral phases grow within the pore structure. The new treatment of the continuum of processes from nucleation to crystal growth and aging is validated on an experimental dataset in which magnesite nucleates and grows as a result of forsterite dissolution in CO2-saturated aqueous solution.

[1] Steefel & Van Cappellen (1990) *GCA* **54**, 2657-2677.