Pore-scale investigation of precipitation driven diffusivity change at column-scale

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Mineral precipitation is observed in many Earth and environmental systems, as a result of changes in environmental conditions (e.g. temperature), injection of oversaturated fluids and mixing, and etc. Mineral precipitation reduces the porosity of the system and modifies transport properties, including permeability and diffusivity. In continuum scale models, the change of transport properties are typically related to porosity change, i.e. the amount of precipitation, by constitutive laws such as Archie's law. However, it has been shown that such continuum scale models may fail to fully capture the evolution of transport properties and the extent of reaction observed in column scale experiments [1]. This discrepancy can be attributed to pore-scale processes and the complex dependence of transport properties on pore structures.

In this study, we aim to examine pore-scale phenomena and their controls on column scale diffusivity change. For our investigation, we follow the experimental conditions of [1], in which celestite precipitation was induced in a compact sand column under diffusion controlled conditions. Pore scale reactive transport simulations are performed using blocks of randomly generated sand packs. Different kinetic pathways, such as transition state theory rate laws and nucleation, are examined to account for uncertainty in precipitation mechanisms. The pore scale simulation results are then used to develop new constitutive relations for continuum scale modeling, in order to capture the experimental observations.

[1] Chagneau, A. *et al*, Mineral precipitation-induced porosity reduction and its effect on transport prarameters in diffusion-controlled porous media. Geochemical Transactions, 2015, 16:13.