# Incorporating mineralogical heterogeneity in pore scale models using a direct numerical simulation approach

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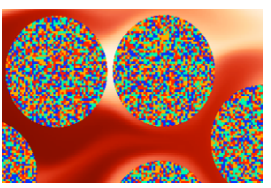
Reactive processes in porous media such as mineral dissolution-precipitation take place at interfaces between fluid and solid phases. Because the different phases are distinguishable at the pore scale, experimental and modeling studies need to consider these interfaces to accurately determine reaction rates. Simulation of reactive processes at the pore scale, however, requires incorporating the complex pore architecture of natural subsurface materials at different spatial scales.

Direct numerical simulation (DNS) of pore scale processes entails the use of conventional discretization methods to solve the governing flow, transport and geochemical equations. In previous work, a Cartesian grid embedded boundary method was developed whereby interfacial surfaces were described by a cut-cell approach [1-3]. This made it possible to simulate pore-scale reactive transport accounting for the surface area available for reaction. Thus, it was possible to treat reactive surface area as a continuum-scale parameter, but also within physically heterogeneous pore domains.

The model is expanded to incorporate mineralogical heterogeneity as characterized by X-ray microtomography or backscattered SEM imaging, and to account for accessibility to reactive mineral phases within the pore domain. Simulations provide insights in how effective rates are develop within natural porous media, especially in understanding the effect of the transport in porous media with a higher degree of textural and mineralogical heterogeneity. Because the various phases dissolving and precipitating are not strictly collocated, transport effects may become more important than in mineralogically homogeneous media.



[1] Molins et al. (2012), *Water Resour. Res.*, 48(3)
[2] Molins et al. (2014), *Environ. Sci. Technol.*, 48(13), 7453
[3] Trebotich et al (2014), *Comput. Sci. Engin.*, 16(6), 22–31