

Multiphase reactive transport modeling – the impacts of two-phase flow on mineral reaction rate

HANG DENG¹, XIN WANG¹, SERGI MOLINS² AND PEI LI³

¹Peking University

²LAWRENCE BERKELEY NATIONAL LABORATORY

³Lawrence Berkeley National Laboratory

Presenting Author: hangdeng@pku.edu.cn

In various subsurface systems, the interactions between multiphase flow and mineral reactions play an important role in controlling the evolution of porous media. These interactions - especially the impacts of multiphase flow dynamics on mineral reaction rates - are rarely accounted for in continuum scale models, or are simply corrected using empirical relationships between reactive surface area and saturation of the aqueous phase. However, these relations used for the correction are not based on pore-scale dynamics.

In this study, we present pore-scale simulations to investigate how mineral reaction rates can be impacted by two-phase flow. For this purpose, we developed a pore-scale multiphase reactive transport model (CrunchFOAM), by coupling the opensource library OpenFOAM with the geochemical capability of CrunchTope using the Application Programming Interface Alquimia. The simulation results of a single channel with different levels of roughness showed that the mineral reaction rate in a gas bubble flow is significantly reduced compared to a single-phase flow system at the same flow rate. The extent of reduction in reaction rate follows a non-monotonic relationship with respect to water saturation, in contrast to the traditionally-used monotonic relationship (i.e., a power law relationship) [1].

We further extend our investigations to pore-doublet geometries, to examine how two-phase flow dynamics arising from competing channels as would be expected in complex porous media affect mineral reaction rates. For our investigations, we control the two-phase flow dynamics by varying the air and water flow rates (i.e., capillary number) and the relative difference between the competing channels. Calcite dissolution rate in these channels is quantified for the two-phase flow cases with different saturations and the corresponding single-phase flow case. The relationships between the changes in dissolution rate in two-phase flow cases and the wetted surface area, the interfacial area, and water saturation are examined to provide insights on improving reaction rate descriptions in multiphase continuum scale models.

[1] Li, P., Deng, H.*, Molins, S., The Effect of Pore-Scale Two-Phase Flow on Mineral Reaction Rates, *Frontiers in Water*, 2022, <https://doi.org/10.3389/frwa.2021.734518>