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Improving Simulation of Mineral Reaction Rates in Porous Media via Enhanced Understanding of Mineral Accessible Surface Area

MD FAHIM SALEK AND LAUREN E. BECKINGHAM

Auburn University

Presenting Author: mzs0184@auburn.edu

Simulating mineral reaction rates in porous media remains challenging, in part due to a lack of understanding of mineral reactive surface area and guidelines for estimating such model parameters. Batch reactor experiments can elucidate details on the kinetics of mineral dissolution and precipitation but have noted limitations for estimating reaction parameters in field systems. In part, these discrepancies stem from mineralogy and pore structure heterogeneities that control flow and reactions in porous media. Using multi-scale 2D and 3D imaging, one can gain advanced understanding of fluid flow in porous media systems and associated mineral surfaces that will be in contact with reactive fluid, or those accessible for reaction. Image obtained accessible mineral surfaces have shown promise as a means of estimating mineral reactive surface area and improving simulations of mineral reaction rates for intact porous media samples. Accounting of the multi-scale nature of pore connectivity, including the possibility for nanopore connectivity, is an important part of identifying effective porosity and accessible mineral surface areas. The extensive time and resources needed to quantify accessible mineral surface areas using this approach is an ongoing challenge. Through analysis of accessible surface areas of numerous sandstone samples, accessibility ratios and predictive relationships between easily measured parameters were explored. Accessibility ratios for quartz, feldspar and carbonate minerals are relatively well constrained (typically <1.5) while those for clay minerals range between 4-16. Accessible surface areas are typically lower than the reported range of mineral specific surface areas and show some dependence on porosity and abundance. Additional data, however, are needed to improve reliability of such relationships where machine learning has shown promise as a way of increasing the speed of image processing. Accurate quantification of the evolution of accessible surface area is additional consideration for improving simulations over long times. Quantification of the reactive evolution of mineral accessible surface area in laboratory dissolution experiments shows the need for improved reactive surface area evolution equations in reactive transport simulations.