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Pore structure control on residence times and coupling of biogeochemical reactions

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Pore structure controls the spatial distribution of microbial activity, the transport of chemical species, and the coupling between biotic and abiotic reactions. An explicit representation of pore geometry allows for a pore-scale reactive transport framework to resolve coupled hydrological and geochemical processes and accurately capture their interactions. However, such simulations are computationally expensive, in particular when resolving detailed microbial metabolism [1], and hence we explore ways to minimize the computational resources required.

To that end, we compare pore scale simulations in two and three dimensions and assess the discrepancies that arise in breakthrough curves and fluid age distributions. Our simulation results show that two-dimensional models systematically underestimate permeability and produce medium-dependent biases in mean travel time and solute spreading. Discrepancies are strongest at low porosity, where out-of-plane flow paths that bypass constrictions are not accounted for in 2D. Nevertheless, as the connectivity in 3D versus in-plane differs between media, 2D slices taken from a 3D medium can predict earlier breakthrough in some geometries yet later breakthrough in others.

In ongoing work, we investigate how pore scale heterogeneity affects the coupling between reactions and different elemental cycles as the strength and location of these interactions have implications how accurately the pore space needs to be resolved. Finally, particularly critical when considering systems with large reaction networks involving many chemicals and microbes (e.g., [2]), we explore the use of the model output as training data for machine learning-based surrogate models [3], and we evaluate to what extent surrogate models can effectively reproduce pore-scale reaction behavior at significantly reduced computational cost.

References:

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