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Understanding pH dependent transport through theory and experiments

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Any reactive transport model at the Darcy scale is inherently empirical, because the complex microstructure of a natural porous material is not known in sufficient detail. The development of an appropriate reactive transport model is therefore always an inverse problem based on the interrogation of the sample through experiments. Experiments don't just parametrize a given model, but they must discriminate between multiple candidate models. In many cases, the robustness of the predictions will depend more on the model choice than the parameterization of the individual models.

The challenge in the design of reactive transport experiments is therefore to conduct suites of experiments that discriminate between different candidate models. This requires identification of experimental conditions where model predictions diverge. Numerical simulations that provide only particular solutions and don't inform the overall behaviour are not well suited for this. In contrast, theory can inform the overall behaviour and therefore guide experimental design. The first-order behaviour of reactive transport with surface complexation is captured by the high Pe-number limit of the governing equations. In this limit, the theory of systems of hyperbolic equations can be used to develop analytical solutions. These solutions highlight the different types of reaction front morphologies and the conditions under which they occur. This allows the construction of a regime diagram and hence informs the overall behaviour of the reactive transport system.

Here we present a well-controlled and well-characterized set of reactive transport experiments with variable pH and salinity in combination with a theoretical analysis of several candidate reactive transport models.

The theoretical analysis highlights conditions at high initial pH and low injected pH where the predictions of different models diverge. This has allowed us to target column flood experiments to distinguish between these candidate models. We can show that the difference in model predictions is not just a quantitative difference in quality of the fit to the experimental data, but some models predict the qualitatively wrong type of reaction front.

We believe that experimental design based on the theory of hyperbolic systems of equations is a powerful tool to identify the appropriate reactive transport model and hence the dominant reactions that control solute transport.