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Reactive transport modelling of water-rock reactions in carbonate systems: comparison of “bottom up” and “top down” approaches and application of explainable machine learning

WENWEN WEI AND FIONA WHITAKER

University of Bristol

Presenting Author: ls19465@bristol.ac.uk

Over the past two decades, the application of reactive transport modelling (RTM) has been central to developing process-based thinking about carbonate diagenesis. However, across disciplines, further advances in the simulating reactive transport in complex natural systems require key challenges to be addressed (Steefel, 2019). We investigated several fundamental challenges of modelling water-rock interaction in carbonates, focussing on (1) the importance of accurate thermodynamic speciation and (2) of considering multiscale processes.

Accurate thermodynamic speciation is critical for modelling water-rock reactions, including carbonate diagenesis, that occur close to equilibrium conditions. Challenges here are rooted in limitations in knowledge of microscopic mechanisms of solute-solvent interactions and difficulties in accurately calculating activity coefficients over a broad compositional range using phenomenological models. Our investigations of the two fundamental approaches: “bottom up” (using phenomenological models to calculate activity coefficients and equilibrium constants) and “top down” (using stoichiometric constants to determine equilibrium state) to thermodynamic speciation suggest that integrating the strengths of different calculation approaches and thermodynamic databases enables an optimized representation of the carbonate, and potentially also other, geochemical reaction systems across a range of temperatures (0~>300 ^{o}C), pressures (1~>1000 bar) and compositions(0~>6 m). This optimized representation requires mapping the multi-dimensional input parameters with outputs which could be achieved only by applying machine learning (ML).

Representing geochemical processes across multiple temporal and spatial scales is a key challenge of modelling carbonate diagenesis and many other geochemical systems. Because of the intrinsic complexity of natural solutions and minerals these problems tend to be highly dimensional, which challenges classical methods but can be addressed using the power of ML. To overcome the inherent ‘black-box’ nature of ML and to effectively model complex multiscale geochemical process, we apply eXplainable Machine Learning (XML). Despite its proven potential for new scientific insight in other disciplines, this approach is rarely considered by the geochemical community. Our results demonstrate how integrating physically-informed ML with XML can create a powerful synergy and enable efficient simulation of multiscale geochemical processes.

We believe that this contribution highlights new approaches to geochemical calculation and modelling that could help to address the leading challenge of modern geochemistry.