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# Adsorption, ion exchange, and surface complexation models for rock-fluid-fluid interactions: an overview and a new implementation in REAKTORO

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The adsorption of ionic species at the interfaces between rock and brine, and between brine and non-aqueous phase liquids (NAPL) such as crude oil, can significantly impact the mobility of these substances in porous media. In this work, we present a set of simple benchmarks to evaluate the accuracy and consistency of existing mathematical models and thermodynamic software in predicting the chemical interactions at these interfaces. We also propose a new open-source implementation of surface complexation models in REAKTORO with practical applications in enhanced oil recovery (EOR), carbon capture and storage (CCS), and ground water remediation. These models, which take the form of Langmuir isotherms in their simplified form, are commonly used to model rock-brine interactions and explain experimental observations such as electrophoretic mobility, streaming potential, and chromatographic retention of ions. However, there is currently no systematic comparison among the various forms of surface complexation models and their numerical implementations. To address this gap, we suggest a range of rock-brine mixtures including natural and artificial calcite, sandstone, and clay minerals in contact with brines of different compositions, and solve these systems using Langmuir, ion exchange, Constant Capacitance (CC), Diffuse Double Layer (DDL), Triple Layer (TL), and Charge-Distribution Multisite Complextion (CD-MUSIC) models in Phreeqc, Geochemists Workbench, Visual Minteq, and ORCHESTRA. We compare the results with our own numerical and analytical solutions. In addition, we present a general formulation of surface complexation models in REAKTORO, addressing issues with the existing numerical implementations related to the explicit calculation of the double-layer composition and the assumptions made about the thickness of the double layer. Our new implementation and benchmarks provide a comprehensive, consistent, and numerically efficient framework for modeling interactions between charged interfaces and their impact on multiphase flow and mechanical behavior in subsurface porous media.

## Participation

In-Person

## References

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