Geochemistry at interfaces: In search of a new modelling approach

MAVRIK ZAVARIN[1*]

[1] Glenn T. Seaborg Institute, Physical & Life Sciences, Lawrence Livermore National Laboratory, Livermore CA 94550, USA (*correspondence: zavarin1@llnl.gov)

The migration of pollutants, nutrients, and carbon in earth systems is often controlled by reactions at solid-water interfaces. Accurate prediction of their migration is critical to nuclear forensics, climate modelling, environmental remediation, nuclear waste disposal, and various other fields. Each of these fields relies on sophisticated reactive transport codes to simulate the fate and transport of relevant constituents (e.g. metals, organic compounds, etc.) in earth systems. These codes, in turn, rely increasingly on mechanistic rather than empirical models to describe constituent interactions. Large databases are used to parameterize these interactions within the simulated domains. These databases often take the form of thermodynamic databases focused on aqueous speciation and mineral precipitation reactions. However, most of these databases have focused on a narrow set of constituents that are relevant to particular fields. Globally, no databases exist that integrate aqueous speciation, mineral precipitation, and reactions at solid-water interfaces (i.e. surface precipitation, surface complexation, ion exchange). As a result, the databases are limited in their applicability to problems requiring the prediction of transport in earth systems.

Development of solid-water interface reaction databases is essential to making progress in simulating reactive transport in earth systems. Their development is hindered by at least three key issues: (1) unidentified processes and limited data for reactions at interfaces (2) a lack of consensus on how to describe solid-water interface reactions and (3) inconsistent parameterization of models used to describe those reactions. As a result, simple compilation of reaction equations from the literature is not possible. Instead, (1) development of a new modelling paradigm for reactions at interfaces, (2) compilation of raw data from the literature, and (3) refitting of data within the context of a new modelling framework are necessary. In this paper, we describe our approach for the case of uranium sorption to quartz.