Development of surface complexation databases for contaminant transport modeling

M. ZAVARIN[1*]

[1]Glenn T. Seaborg Institute, Lawrence Livermore National Laboratory, Livermore, CA 94551 USA (*correspondence: zavarin1@llnl.gov)

The need to develop self-consistent surface complexation databases for nuclear waste repository performance assessment was identified many years ago [1] and was expressly identified in the recent NEA Sorption project reports [2, 3]. In principle, these databases could be applied to a wide range of environmental contaminant transport problems outside the nuclear waste arena as well. However, significant progress in developing such databases has been slow. Some progress has been made only recently in various international nuclear waste repository programs [4-6]. Nevertheless, the best path forward for developing such databases remains an open question [6].

Three key issues that prevent our development of surface complexation databases include (1) an inability to integrate disparate data sets and surface complexation model constructs into single unified model, (2) an inability to produce self-consistent reaction constants based on a common set of aqueous speciation constants and surface properties (3) the absence of error propagation in fitting routines and databases to assess paramater uncertainties.

We recently developed a test-case for U(VI) sorption to quartz and demonstrated how a self-consistent set of surface complexation constants could be produced from ~400 batch sorption data digitized from the published literature. When linked to a parameter estimation software [7], parameter uncertainties, covariances, and sensitivities could be extracted. Thus, it appears that this approach can provide a robust path forward for database development. Importantly, the approach provides a platform for testing various surface complexation models and assess their ability to capture observed sorption data in a comprehensive manner. However, effort required to build such a comprehensive database and questions of data quality propagation must still be resolved.

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