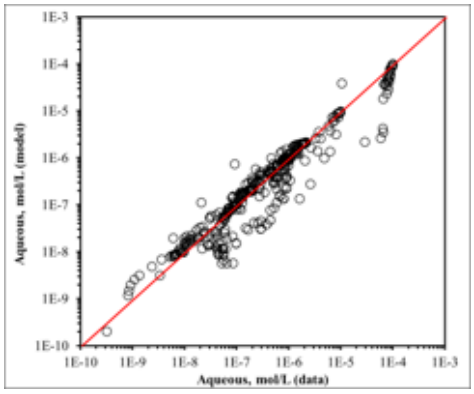
Mineral-water databases for use in radionuclide transport simulations

M. ZAVARIN [1*]

[1]Glenn T. Seaborg Institute, Lawrence Livermore National Laboratory, Livermore, CA 94551 USA

The need for surface complexation models for nuclear waste repository performance assessment was identified many years ago[1]. However, the best path for developing such databases remains an open question[2]. One approach, though somewhat painful, is to digitize raw sorption data available in the literature and develop models that capture sorption across the widest possible range of solution conditions in a comprehensive manner.



We have begun developing such an approach. References from the RES^{3}T database (Helmholtz Zentrum Dresden Rossendorf) are being digitized and data fitting routines developed using a combination of (1) PHREEQC geochemical code, (2) PEST parameter estimation software [3], and (3) LLNL thermodynamic database combined with the NEA Themchemical database effort. A critical component to this effort is the quantification of data uncertainty. A test-case for U(VI) sorption to quartz demonstrates how a self-consistent set of surface complexation constants could be produced from ~500 batch sorption data digitized from the published literature (Figure 1). The approach provides a platform for testing various surface complexation models and assess their ability to capture available sorption data. This approach can provide a robust path forward for database development. However, success necessitates community involvement in data digitization efforts.

[1] Bradbury et al. (1993) J Col Interf Sci **158**, 364-371. [2] Geckeis et al. (2013) Chem Rev **113**, 1016-1062. [3] Doherty (2003) Watermark Numerical Computing.