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AQUA-MER Aqueous Speciation Database: A Web Resource for Multi-Scale Modeling of Mercury Biogeochemistry

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Multi-scale geochemical modeling is important for predicting the fate of metals in terrestrial surface and subsurface systems. Typically, experimentally determined stability constants (i.e., log *K*) are used to calculate speciation profiles and to predict transport and transformations in the environment. However, modeling mercury (Hg) biogeochemistry suffers from a lack of reliable experimental data. For instance, experimentally measured log *K* values for $Hg(Cys)_2$ vary by 10-20 log units. Furthermore, the log *K* value for aqueous HgS was not measured directly but was derived by extrapolating the values for CdS and ZnS. Uncertainty in log *K* values propagates nonlinearly through speciation models of aqueous chemical systems. Latin hypercube sampling from a normal distribution of log *K* values leads to highly skewed distributions of aqueous Hg-containing species concentrations. Thus, if uncertainty is not considered, speciation model output of concentrations deviate away from the modes of the distributions, or values of the highest probability. Quantum chemical calculations can be used to supplement missing thermodynamic data. We have developed protocols to calculate accurate thermodynamic constants for environmentally relevant molecular species. We have developed an aqueous Hg speciation database, *AQUA-MER*, which collects high-quality experimental data adherent to IUPAC standards, accurate computational data, and provides a web interface to perform multi-scale Hg biogeochemical modeling. Currently, the database includes three modules: experimental log *K* data, calculated log *K* data, and Hg speciation modeling. The Hg speciation module currently uses PHREEQC to calculate aqueous speciation profiles using thermodynamic constants from experimental data, computational data, or both. Further refinement of the database will provide a one-stop website for multi-scale Hg biogeochemistry studies. Future studies will focus on combining the atomistic models with a macroscopic continuum-scale modeling framework to predict the transport and transformation of Hg in the environment.