Developing and Using Kinetics Databases in Environmental Chemistry

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Over the past several decades, researchers in the environmental sciences have produced large quantities of data detailing the kinetics of environmentally relevant chemical processes. A characteristic of this data set, in addition to its size, is the variety of temporal and length scales that are encompassed. Studying the fate of an aqueous contaminant, for example, could entail spectroscopies that examine precise molecular arrangements under rarefied conditions, bench-top kinetics experiments that examine a few of the myriad chemical transformations that occur in the environment, and field studies that examine environmental processes as a whole, but, with minimal control over the relevant variables. Databases of kinetics information provide an ideal tool for synthesizing this sort of cross-scale data into a knowledge base that can be used to predict the behavior of environmental systems and to diagnose the quality of the accumulated data. In this talk we describe the development of kinetics databases within Penn State's Center for Environmental Kinetics Analysis and the use of these databases in modeling mineral weathering processes and parameterizing rate laws for dissimilatory metal reducing bacteria activity. Topics that will be addressed include: (i) automated harvest of graphical, tabular, and textual information for compilation of legacy data, (ii) implementation of ontologies and ontology mapping schemes for enabling effective searches, and (iii) incorporation of analysis and modeling tools for ready use of the database.