MinKin: A new computational tool for modeling the kinetics of multi-component geochemical systems

D. R. HUMMER[1] AND P. J. HEANEY[2]

[1]Department of Earth, Planetary and Space Sciences, University of California Los Angeles, Los Angeles, CA, dhummer@epss.ucla.edu

[2]Department of Geosciences, The Pennsylvania State University, University Park, PA, pjheaney@psu.edu

Understanding the kinetics of mineral-fluid reactions often involves fitting rate laws to a time-series of experimental concentration data in order to extract rate constants for individual reactions. However, the natural systems of interest to geochemists often involve multiple mineral phases reacting with components of a fluid phase, making it intractably complex to solve the system's differential equations (i.e., rate equations) and fit them to concentration data. Here we present MinKin (for "Mineral Kinetics"), a global optimization code for Matlab capable of fitting a standard chemical kinetic model to experimental concentration data even in the absence of solutions to the system's kinetic equations. MinKin allows users to specify the species and reactions of a geochemical system consisting of a fluid with up to two aqueous species and up to three mineral species, and then uses the global optimization algorithm of Differential Evolution (DE)1,2 to calculate the rate constants that minimize the error between the model and the data. Trial calculations reveal that MinKin is able to simultaneously and correctly calculate up to six rate constants on a time scale of minutes, with an accuracy of roughly the same magnitude as that of the input data. This makes MinKin a novel and powerful way to analyze the kinetics of multi-component geochemical systems, especially for systems that are intractable by any other method.

[1] R. Storn, K. Price. (1997) *J. Global Optimization* **11,** 341-359. [2] K. Price, R. Storn. (1997) *Dr. Dobbs Journal* **22**(4), 18-24.