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Computational methods for multiphase equilibrium and kinetics calculations for geochemical and reactive transport applications

Allan Leal and Martin Saar
Institute of Geophysics, ETH Zurich, Zurich, Switzerland (allan.leal@erdw.ethz.ch)

Computational methods for geochemical and reactive transport modeling are essential for the understanding of many natural and industrial processes. Most of these processes involve several phases and components, and quite often requires chemical equilibrium and kinetics calculations. We present an overview of novel methods for multiphase equilibrium calculations, based on both the Gibbs energy minimization (GEM) approach and on the solution of the law of mass-action (LMA) equations. We also employ kinetics calculations, assuming partial equilibrium (e.g., fluid species in equilibrium while minerals are in disequilibrium) using automatic time stepping to improve simulation efficiency and robustness. These methods are developed specifically for applications that are computationally expensive, such as reactive transport simulations. We show how efficient the new methods are, compared to other algorithms, and how easy it is to use them for geochemical modeling via a simple script language. All methods are available in Reaktoro, a unified open-source framework for modeling chemically reactive systems, which we also briefly describe.