



Coupling Gibbs minimization to reactive transport models

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Fluid flow processes below the Earth's surface play an important role in many geological settings, from shallow depths in aquifers and hydrocarbon reservoirs down to tens of kilometers, where subduction of oceanic crust brings fluids to large depths. Industrial applications, environmental studies as well as fundamental geological research depends on accurate description and understanding of fluid flow, mass transport and reaction in rocks. Numerical modeling of fluid flow and reaction through rocks is a powerful tool to understand and interpret geological field observations as well as for predicting large scale geodynamic processes, hydrocarbon migration, CO₂ storage reliability, formation of economic ore deposits, and subsurface contamination, to name just a few. In all these cases it is important to have powerful predictive modeling tools that can run in sufficiently high resolution to capture the physical processes on a large variety of scales, both in time and space.

Chemical reactions and fluid flow are intimately linked and have to be solved in a coupled way to accurately and consistently model the geological processes. To date, the usual approach in most reactive transport modelling consists of solving non-linear system of chemical reactions at each grid node in the model domain. Here, we explore the use of Gibbs minimization for solving chemical reactions and fluid flow in a coupled system.

We apply our method to dehydration of serpentinite during subduction processes. Dynamic porosity, density, and fluid pressure evolution are coupled to reactions by precomputing tens of thousands of phase diagrams covering P-T and compositional space. We compare the results of two approaches: solving individual reactions versus Gibbs minimization using precomputed look-up tables. Both approaches give similar results, however, the Gibbs minimization approach allows for including most complex solid and fluid solution models, whereas in the reaction approach this is very cumbersome. Additionally, we explore the relation between activity/chemical potential diagrams, and isochemical phase diagram sections and evaluate their usage in reactive transport models.