An Integrated Thermodynamic and Dynamic Approach to Modeling High Temperature Fluid Interaction in the Mantle Wedge

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Melting in the mantle wedge beneath volcanic arcs is generally considered to be driven by fluids extracted from the down-going plate. However, how these fluids are transferred to the hot mantle wedge is largely unknown. Attempts to model this process have been challenged by the strong coupling between fluid-rock reaction and transport dynamics which means that neither the dynamics nor the chemical evolution can be considered in isolation. Here we present a new computationally tractable framework, based on the concepts of non-equilibrium thermodynamics, that holistically integrates thermodynamics and fluid dynamics. We apply this framework to model the interaction of high temperature super-critical fluids with the mantle wedge in the Mg$_2$SiO$_4$-SiO$_2$-H$_2$O and Mg$_2$SiO$_4$-SiO$_2$-K$_2$O subsystems. The model employs a thermodynamically consistent generalization of the viscous two-phase flow equations that allows for multiple solid and liquid phases. By rephrasing the thermodynamics in terms of a set of independent reactions, and using chemical affinity of each reaction as a scalar measure of disequilibrium, we avoid having to do computationally expensive free-energy minimization on the fly. Thermodynamic models are only required to return thermodynamic quantities including chemical potential, specific entropy, density and heat capacity. The coupled evolution of phase proportion, fluid composition, fluid and bulk solid velocity fields and temperature can then be tracked at reduced computational cost. We use this model to explore the effects of fluid composition, the extent of local chemical disequilibrium and temperature gradient on flow focusing and the resulting evolution of fluid composition. This work is part of the ENKI project which is developing computational thermodynamics tools which support the development and calibration of thermodynamic models and the integration of these models into fluid dynamics codes. We will describe the ongoing development of the computational infrastructure which will allow the approach outlined here to be extended to more complex systems to support future study of fluid-rock interactions in subduction zones.