



Numerical Modelling of Multi-Phase Multi-Component Reactive Transport in the Earth's interior

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We present a conceptual and numerical approach to model processes in the Earth's interior that involve multiple phases that simultaneously interact thermally, mechanically and chemically. The approach is truly multiphase in the sense that each dynamic phase is explicitly modelled with an individual set of mass, momentum, energy and chemical mass balance equations coupled via interfacial interaction terms. It is also truly multi-component in the sense that the compositions of the system and its constituent thermodynamic phases are expressed by a full set of fundamental chemical components (e.g. SiO_2 , Al_2SiO_5 , MgO , etc) rather than proxies. In contrast to previous approaches these chemical components evolve, react with, and partition into, different phases with different physical properties according to an internally-consistent thermodynamic model. This enables a thermodynamically-consistent coupling of the governing set of balance equations. Interfacial processes such as surface tensions and/or surface energy contributions to the dynamics and energetics of the system are also taken into account.

The model presented here describes the evolution of systems governed by Multi-Phase Multi-Component Reactive Transport (MPMCRT) based on Ensemble Averaging and Classical Irreversible Thermodynamics principles. This novel approach provides a flexible platform to study the dynamics and non-linear feedbacks occurring within various natural systems at different scales. This notably includes major- and trace-element transport, diffusion-controlled trace-element re-equilibration or rheological changes associated with melt generation and migration in the Earth's mantle.