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 simultaneously interacting thermally, mechanically and chemically. This 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 constituting minerals are expressed by a full set of major elements, 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 tension and/or surface energy contributions to the dynamics and energetics of the system are also taken into account.

Our model describes the dynamic evolution and non-linear feedbacks of complex geochemical processes governed by Multi-Phase Multi-Component Reactive Transport (MPMCRT), such as melt generation, migration and differentiation. This novel approach provides a flexible platform to track changes in the chemical compositions and physical properties of the lithospheric mantle through time, over different spatial scales and from various geodynamic environments. It notably includes major- and trace-element transport, diffusion-controlled trace-element re-equilibration and rheological changes associated with melt migration, metasomatism and metamorphism, which is especially relevant to handle the diversity of fluid and melt sources and to simulate the intricate interplay between tectonics and magmatism, characteristic of subduction zones.