

## Connecting forward modeling of thermo-chemical mantle convection in a 3-D spherical shell to observational constraints

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In recent mantle convection simulations it is possible to simulate thermal-chemical-phase structures including complicated processes such as self-consistently calculated mineral phase relationships, melt-induced crustal formation and extremely large variations of viscosity based on laboratory rheological experiments. Here we introduce several examples of numerical simulations of thermo-chemical, multiphase, compressible mantle convection in a 3-D spherical shell with a self-consistently calculated mineral physics and plate-like behavior.

Results are linked to four observationally- or experimentally-derived quantities: 1. Spectral heterogeneity maps (i.e., lateral spectra versus depth) evaluated from global seismic tomographic inversions, 2. regional radial profiles of shear-wave velocity obtained from waveform analyses, 3. heat flux and variations of heat flux across the core-mantle boundary (CMB) and its relationship to shear-wave velocity anomalies, and 4. the conversion factor between density and shear-wave anomalies obtained from mineral physics [Karato and Karki, 2001].

It is straightforward to match the dominant lengthscales of seismic tomographic inversions, but thermo-chemical convection models typically predict strong heterogeneity that extends over more of the deep mantle than obtained in seismic inversions, implying that the amount of compositional layering above the CMB is relatively small [Nakagawa et al., 2009]. It is, however, possible to explain 1-D shear-wave structures inverted from surface wave data [Khan et al., 2009] using seismic structure calculated from thermo-chemical mantle convection simulations, which predict a stratification of the mean composition in the transition zone and from the upper to lower mantle. The scaling of CMB heat flux to deep mantle seismic shear wave velocity is nonlinear and possibly non-unique, which is important for geodynamo simulations in which heat flux variations are imposed [Nakagawa and Tackley, 2008]. The conversion factor between density and shear-wave anomalies is also a complicated relationship, which should have spatial dependence.

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