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Deep mantle thermo-chemical dynamics in 3D spherical geometry incorporating a realistic phase diagram calculated by free energy minimization

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Deep mantle dynamics and the resulting thermo-chemical-phase structures are here studied using thermo-chemical mantle convection simulations in a 3D spherical shell that incorporate composition-dependent phase diagrams calculated by free energy minimization. This improves on our previous studies, which used simple depth-dependent thermodynamic properties and calculated seismic anomalies based on linearized derivatives around a pyrolitic mean composition. Realistic mineral assemblages of mantle rocks have several high pressure and temperature phases, which vary substantially as composition changes from MORB-like to harzburgitic. Linearized treatments probably do not adequately capture the variation of physical properties with composition and temperature. In order to get closer to a realistic mineralogy, we here calculate composition-dependent mineral assemblages and their physical properties using the code PERPLEX, which minimizes free energy for a given combination of oxides as a function of temperature and pressure, and use the resulting properties in a 3-D spherical numerical model of thermo-chemical mantle convection, with three-dimensionally-varying physical properties [Nakagawa et al., 2007 in Goldschmidt conference]. Preliminary results are that while thermo-chemical structures are not greatly different from in the previous treatment, the spectral profiles of seismic anomalies seem to match seismic tomographic models more closely. Here we extend these results to focus on seismic signatures of the deep mantle including the post-perovskite phase transition. There is still uncertainty in the thermodynamic prop-

erties of the post-perovskite phase; hence the phase relationship of post-perovskite and its composition-dependence is treated as ‘adjustable’ within mineral physics uncertainties. The thermal-chemical-phase structures in our latest numerical simulation models are compared to the latest seismologically-observed structures.