



Dynamic and seismic expressions of mineral phase transitions in mantle circulation models computed with TerraNeo

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One major objective in geodynamics is to create models of mantle flow that provide quantitative information to other Earth science disciplines. In this respect, geologically informed fluid dynamics simulations, such as mantle circulation models (MCMs) are a key component. In addition, thermodynamic models of mantle mineralogy are essential in that they can provide detailed information on material behaviour, such as density, thermal expansivity, elastic parameters and specific heat capacity, as a function of pressure and temperature for the geodynamic simulations. They are also required in the assessment of the MCMs to link temperatures to seismic velocities and density. This way, a number of secondary predictions, such as seismic, geodetic and geologic data, can be computed, which enables the validation of our models and the testing of geodynamic hypotheses by comparison to observations.

Here, we focus specifically on the dynamic effects and seismic imprint of the mantle transition zone (TZ). The complex set of phase transformations, together with an increase in viscosity, in this depth range is expected to influence vertical mass flow between upper and lower mantle. Still, neither the associated dynamic effects nor the seismic structure of the TZ have conclusively been constrained to date. Using our highly scalable new mantle convection software TerraNeo, based on the matrix-free finite-element framework HyTeG, we present a suite of MCMs with different formulations of compressibility. Classically, compressibility is included in the mantle convection simulations in form of the truncated anelastic liquid approximation (TALA), and the effects of phase transformations are either neglected or incorporated in parametrized form at constant depth. A physically more complete treatment of compressibility has recently been introduced in the form of the 'Projected Density Approximation' (PDA; Gassmöller et al., 2020). The PDA is based on tabulated material properties from the thermodynamic mineralogical models, thus allowing us to self-consistently capture non-linear buoyancy effects specifically due to phase transitions in the simulation. Comparing MCMs using TALA and PDA, we will highlight effects of mineral phase transitions on the evolution of mantle flow over time, the resulting present-day temperature field, as well as its seismic signature.