Three-dimensional numerical simulations of thermo-chemical multiphase convection in the Earth's mantle

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Abstract

Three-dimensional numerical simulations of thermo-chemical mantle convection that include melting-induced compositional differentiation, self-consistent plate-like behavior, and composition-dependent solid–solid phase changes (including the newly-discovered post-perovskite transition) are used to model the 4.5 billion year evolution of the Earth, and are successful in matching many of the major observational constraints. These simulations are at high Rayleigh number (10^7) and large viscosity contrast (varying by six orders of magnitude with temperature and two orders of magnitude with depth), and can match many characteristics of Earth's mantle from a compositionally-homogeneous initial condition, with all chemical heterogeneity generated by melting-induced differentiation. Such simulations achieve greater realism than previously possible and facilitate an improved understanding of the dynamics of the Earth and planetary interiors.

Keywords: Mantle convection; 3D numerical simulations; Melt-induced differentiation

1. Introduction

Three-dimensional numerical simulations of mantle convection with both thermal and chemical buoyancies have been published by only two groups. The Cartesian geometry calculations of Tackley [1,2] characterized the three-dimensional structures and their observational signatures that are obtained when a dense layer of compositionally-distinct material is present at the base of the mantle. This line of investigation was extended to spherical-shell geometry by McNamara et al. [3]. In these studies, a compositionally-dense layer was inserted as an initial condition, with no consideration given as to how it originated. Such a layer would most likely originate as a result of the segregation and settling of dense crustal material generated by partial melting in the shallow mantle, after it has been subducted into the Earth's interior, and this mechanism has been modeled in the two-dimensional calculations of Christensen et al. [4], Tackley et al. [5] and Xie et al. [6]. The latter two studies, as well as Ogawa [7], also included a yield stress rheology that leads to self-consistent plate tectonic-like behavior, as discussed by Moresi et al. [8] and Tackley [9]. Thus, numerical simulations of mantle convection that include both melt-induced compositional differentiation and self-consistent plate tectonic-like behavior have been performed only in two dimensions. Here, we present a three-dimensional calculation that includes these two complexities, and additionally present one that incorporates the post-perovskite transition, newly-discovered by Oganov et al. [10] and Murakami et al. [11], that occurs near the base of the mantle.

The inclusion of these complicated processes is important for understanding the dynamics, evolution and structure of the Earth's interior, but makes three-dimensional modeling challenging.

2. Numerical procedure

The code STAG3D, which uses a finite-volume multigrid solver for the flow field and tracers for composition, is used to study thermo-chemical mantle convection including self-consistent plate-like behavior, melt-induced compositional differentiation and multi-

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component phase changes in a two- or three-dimensional Cartesian box with an aspect ratio of four. The physical model and numerical procedure are detailed in previous works by Tackley [1,2] and Tackley et al. [5,12]. The infinite Prandtl number and compressible anelastic approximations are used, as is common in mantle convection studies. An impermeable, free-slip and isothermal boundary condition is applied to both top and bottom boundaries, with periodic side boundaries. The temperature of the bottom boundary is adjusted each timestep to account for the cooling of the core due to heat conducted into the mantle:

$$dT_b/dt = -KF_b \tag{1}$$

where T_b is the temperature at bottom boundary, K is the cooling constant and F_b is the heat flux across the bottom boundary. The viscosity η is based on a Bingham type formulation, as in Stein et al. [13], which is strongly dependent on temperature, depth and yield stress:

$$\eta = \left(\frac{1}{1/\eta_d + 1/\eta_y}\right)^{-1} \tag{2}$$

$$\eta_d = \eta_0[1 + 29H(0.7716 - z)]\exp(4.6z)\exp\left[\frac{27.631}{T + 0.88}\right] \tag{3}$$

$$\eta_y = 10^{-2} + \frac{\sigma_y(z)}{2\dot{e}^2} \tag{4}$$

$$\sigma_y(z) = 10^5 + 4 \times 10^5(1 - z) \tag{5}$$

where η_d is the ductile viscosity, η_y is the yielding viscosity, z is the vertical coordinate, H is the Heaviside step function, T is temperature, $\dot{e}$ is the second invariant of the strain rate tensor, and $\sigma_y(z)$ is the yield stress as a function of depth. Since a minimum cutoff of 0.01 is applied to the yielding viscosity (Eq.(4)), this approach can avoid the numerical instability that is often caused by large viscosity variations across a grid cell due to pseudo-plastic deformation. All physical parameters used in this study are listed in Table 1. The physical parameters for the multi-component phase changes are listed in Table 2 of Tackley et al. [10] and those for the post-perovskite transition in Table 1 of Nakagawa et al. [14]. A numerical resolution of 128 (x) × 128 (y) × 64 (z) cells is used, with 16 tracers on each grid cell to track composition.

3. Results

Two cases are presented, one with and one without the recently discovered post-perovskite phase change near the bottom of the mantle. Both cases were run for a simulated time of 4.5 Gyr (0.0118 nondimensional), which takes about two weeks to run on four Intel Xeon 2.4-GHz processors and four days using 16 Intel Pentium 4 3.2-GHz CPUs. The numerical solver is able to converge to stable solutions over this long computational time despite the large variations in viscosity.

Table 1
Physical parameters: $Ra_0 = \rho_0 g \alpha_0 \Delta T_{sa} d^3/\kappa_0\eta_0$ and $K = 3\rho_m c_m d/\rho_c c r_{CMB}$

Symbol	Meaning	Non-D. value	Dimensional value
Ra_0	Rayleigh number	10^7	N/A
ρ_0	Reference (surface) density	1	3300 kg m^{-3}
g	Gravity	1	9.8 m s^{-2}
α_0	Reference (surface) thermal expan.	1	5×10^{-5} K^{-1}
κ_0	Reference (surface) thermal diffusion	1	7×10^{-7} m^{2}s^{-1}
ΔT_{sa}	Temperature scale	1	2500 K
T_s	Surface temperature	0.12	300 K
L_m	Latent heat	0.2	6.25×10^5 J kg^{-1}
τ	Half life	0.00642	2.43×10^9 years
K	Cooling coefficient	1.8	N/A

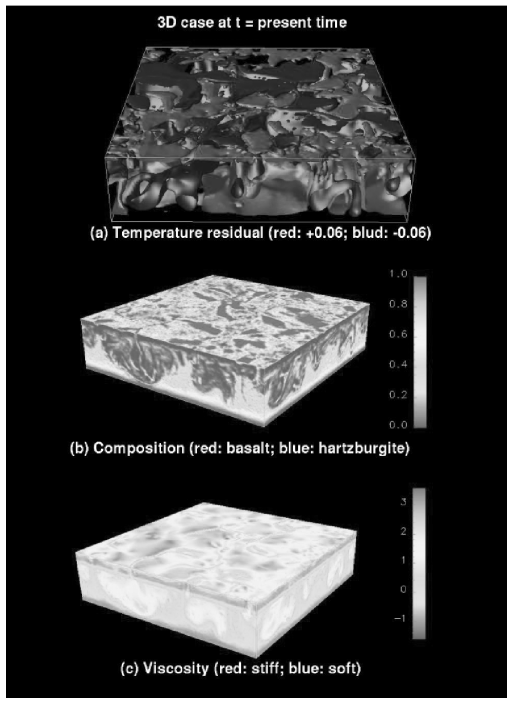

Fig. 1. Temperature (a), composition (b) and viscosity (c) for the case with no post-perovsite phase transition.

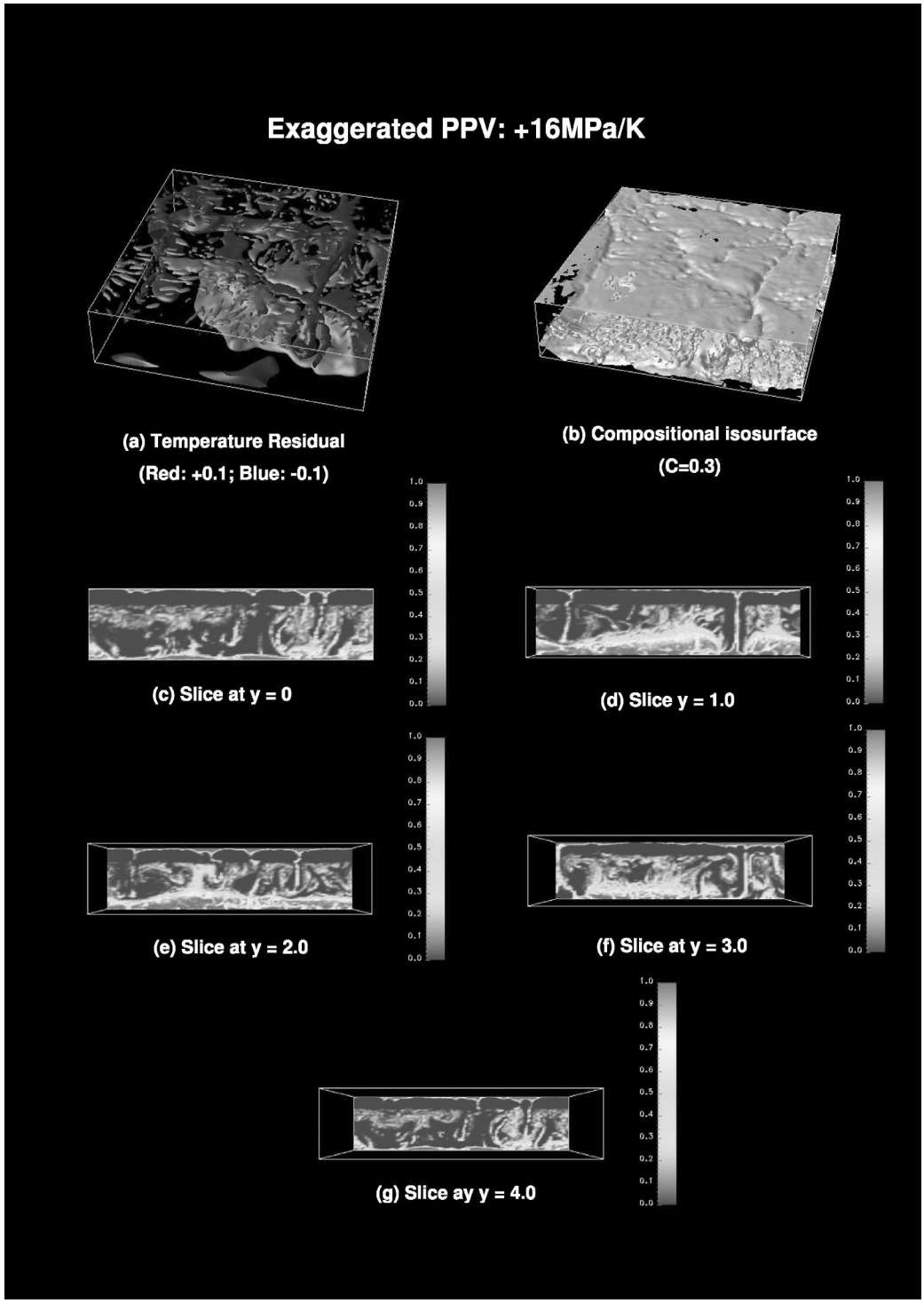

Fig. 2. Temperature isosurfaces (a), composition isosurface (b), and temperature slices (c)–(g) for the case that includes the post-perovskite phase change.

Figure 1 shows the temperature, composition and viscosity fields for the case without the new phase change. Subducted downwelling slabs generate heterogeneous features in the compositional field in the bottom region. Figure 2 shows the same fields for a case in which only the olivine-component phase changes are included but the post-perovskite phase change is added. The lower boundary layer is destabilized and a longer wavelength flow pattern is set up.

4. Conclusions

Numerical simulations of thermo-chemical mantle convection including plate-like behavior and melting-induced compositional differentiation and stratification can now be modeled in three dimensions using STAG3D, a finite-volume multigrid numerical code with a tracer treatment of composition. The solver is stable with large variations in viscosity over long integration times and useful three-dimensional calculations can be done in days to weeks using a small cluster of commodity Pentium-type processors. This will facilitate greater understanding of the mantle dynamics of Earth and other planets. The next step is to move to the more realistic spherical three-dimensional geometry, a suitable code for which is being developed by Hernlund et al. [15].

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