

# Mass transport mechanism between the upper and lower mantle in numerical simulations of thermochemical mantle convection with multicomponent phase changes

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## Abstract

Numerical simulations of thermochemical mantle convection are used to investigate the influence of multicomponent phase changes on mass transport between the upper and lower mantle. The model includes both olivine and pyroxene–garnet components based on a pyrolite composition. The simulations reveal large and focused upwellings through the 660-km phase boundary in the vicinity of subducting slabs. The upwellings are composed of depleted harzburgitic material, which contributes to the depletion of the upper mantle and may generate distinct reservoirs of trace elements in the upper and lower mantle as well. The position and composition of the upwelling is attributed to the development of compositional stratification at the top of the lower mantle, where dense harzburgitic material underlies enriched basaltic material due to a density inversion in the combine phase system. Subducting slabs disrupt the stratification in the vicinity of subduction, permitting a counter flow of harzburgitic material into the upper mantle. This behavior is not observed in a pure olivine phase system, suggesting that realistic mantle compositions are needed to assess the generation of distinct reservoirs in mantle convection simulations. Phase transitions in a multicomponent system provide a plausible mechanism for explaining the formation of a depleted reservoir in the upper mantle without implementing dehydration-induced melting and differentiation in the transition zone.

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**Keywords:** multicomponent phase change; transition zone; thermochemical convection; geochemical reservoirs; counter flow; harzburgite

## 1. Introduction

The role of the transition zone on the dynamics of the mantle has been studied using numerical convection models [1–11], seismic tomography [12,13] and high-pressure experiments [14–19].

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Two- and three-dimensional numerical convection models show that an endothermic phase change in a pure olivine system can induce double-layered mantle convection and generate the episodic overturn (‘mantle avalanche’) [1,2,5–7]. The endothermic phase boundary can also act as a filter to dense material, which becomes entrained in upwelling plumes [4,20]. More general numerical models of thermochemical mantle convection, which include melt-induced differentiation and a realistic composition (based on a pyrolite composition of 60% olivine and 40% pyroxene), have shown that depleted harzburgite material accumulates below basaltic material near the 660-km phase transition [9–11]. This compositional stratification is the result of a density inversion in the combined olivine and pyroxene–garnet systems because these minerals transform to perovskite structure at different depths (see link Fig. 1 in [10]). Several consequences of the density inversion in the olivine and pyroxene systems were anticipated from high-pressure experiments [16,17,19]. However, these previous studies did not quantify the influence of compositional stratification on the transport of mass between the upper and lower mantle.

Here, we investigate the dynamics of the transition zone and uppermost lower mantle using a numerical model of thermochemical mantle convection that includes melt-induced differentiation and multicomponent phase changes. The complex interaction of multiple phase boundaries with upwelling plumes and subducting slabs are analyzed and compared to other interpretations arising from mineral physics experiments. While previous numerical models in single-component systems [21,22] have shown that phase transitions can affect slab dynamics, our primary focus is on the effects of material differentiation on transport through the 660 km depth. We also compare the role of phase transitions to a simple theory for dehydration-induced differentiation [23] because that mechanism is another possibility for generating depleted reservoir in the upper mantle.

## 2. Model description

A numerical code STAG3D is used to study thermochemical mantle convection in a two-dimen-

sional half cylindrical shell [10,11,24]. The anelastic approximation is used with the assumption of infinite Prandtl number. The viscosity is temperature-, depth- and yield-stress-dependent given as

$$\eta_d(T, z) = \eta_0 [1 + (\Delta\eta - 1)H(0.7716 - z)] \exp[4.6z] \times \exp\left[\frac{27.631}{T + 1 - T_s}\right]$$

$$\sigma_Y(z) = \sigma_b + \sigma_d(1 - z)$$

$$\eta(T, z, \dot{\epsilon}) = \min\left(\eta_d(T, z), \frac{\sigma_Y(z)}{2\dot{\epsilon}}\right) \quad (1)$$

where  $\eta_d(T, z)$  is the ductile viscosity,  $\Delta\eta$  is the viscosity jump between upper and lower mantles,  $H$  is the Heaviside step function,  $\sigma_Y(z)$  is the depth-dependent yield stress,  $\sigma_d$  is the yield stress gradient,  $\sigma_b$  is the yield stress at the surface,  $\dot{\epsilon}$  is the second invariant of the strain rate tensor,  $T_s$  is the surface temperature, and  $z$  is the vertical coordinate, which varies from 0 at the CMB to 1 at the surface. In this formulation, the viscosity changes by six orders of magnitude with temperature, two orders of magnitude with depth (although the increase along an adiabat is less), and  $\Delta\eta=30$  across the 660-km discontinuity.

Table 1  
Mantle model physical mantle parameters

Symbol	Meaning	Nondimensional value	Dimensional value
$Ra_0$	Rayleigh number	$10^7$	N/A
$\eta_0$	Reference viscosity	1	$1.4 \times 10^{22}$
$\Delta\eta$	Viscosity jump at 660 km	30	N/A
$\sigma_b$	Yield stress at surface	$1 \times 10^5$	117 MPa
$\sigma_d$	Yield stress gradient	$4 \times 10^5$	$162.4 \text{ Pa m}^{-1}$
$\rho_0$	Reference (surface) density	1	$3300 \text{ kg m}^{-3}$
$g$	Gravity	1	$9.8 \text{ m s}^{-2}$
$\alpha_0$	Ref. (surface) thermal expan.	1	$5 \times 10^{-5} \text{ K}^{-1}$
$\kappa_0$	Ref. (surface) thermal diff.	1	$7 \times 10^{-7} \text{ m}^2 \text{ s}^{-1}$
$\Delta T_{sa}$	Temperature scale	1	2500 K
$T_s$	Surface temperature	0.12	300 K
$L_m$	Latent heat	0.2	$6.25 \times 10^5 \text{ J kg}^{-1}$
$\tau$	Half life	0.00642	2.43 Gy
$v$	Velocity	1310.65	1 cm/y

$$Ra_0 = \rho_0 g \alpha_0 \Delta T_{sa} d^3 / \kappa_0 \eta_0.$$

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