Living dead slabs in 3-D: The dynamics of compositionally-stratified slabs entering a “slab graveyard” above the core-mantle boundary

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Abstract

Segregation of subducted mid-ocean ridge basalt (MORB) at the CMB has been identified as a potentially important mechanism in the long-term evolution of the mantle and core. Here, three-dimensional (3-D) and two-dimensional (2-D) simulations of a compositionally-stratified slab reaching the CMB are presented, with the goals of characterising the resulting thermo-chemical structures for comparison with seismic studies, and of quantifying the fraction of MORB that is able to segregate and remain near the CMB. Compositional stratification of the slab results in a strong torque due to the relatively high density of basalt and low density of harzburgite, which tends to rotate the slab such that the basalt side faces down. Slab-CMB interaction is characterised by heating up of the slab followed by separation of the basalt and harzburgite layers, with harzburgite rising in vigorous plumes. Plumes form at the edges and sides of slabs at the CMB as well as in their interiors (as previously observed for purely thermal slabs) with plume heads dominated by depleted harzburgitic material (sometimes with small amounts of entrained basalt), while plume tails entrain basaltic material. Segregation of basalt depends strongly on the presence or absence of a preexisting dense layer at the CMB and by dimensionality. A preexisting dense layer greatly increases the fraction of basalt that segregates from the slab: in 3-D this fraction is in the range 0.5–0.7 with a layer present compared to 0.25–0.45 with no preexisting layer. Two modes of basalt segregation are observed for slabs that land basalt side-up (i) hot harzburgite extruding from the sides and edges and (ii) hot, harzburgite-rich plumes bursting through the basalt layer (as previously observed in laboratory experiments), whereas for a slab that lands basalt side down (iii) hot basalt can peel off from its underside, displaying fingering instabilities in 3-D. Furthermore, basalt–harzburgite segregation is sometimes observed in slab segments that have already been heated at the CMB and risen a few hundred km, by a folding mechanism. A range of “interesting” structures are observed in the model CMB region, which may be useful in interpreting seismic observations. Strong lateral gradients in composition and temperature are quite common. Structures include plumes next to vertical slab segments, inverted slab sections perched above the CMB and harzburgite curtains. The presence of a stratified layer above the CMB, as observed in global simulations in which a layer builds up by basalt segregation, strongly suppresses plume formation. 2-D simulations give a good first-order guide to the dynamics obtained in fully 3-D geometry, but inherently 3-D structures are missed (plumes versus sheets, fingering) and there is a quantitative difference in the fraction of basalt segregated.

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1. Introduction

The core-mantle boundary (CMB) region has attracted great interdisciplinary interest for many years, and is thought to be a region where thermal, compositional and mineralogical phase effects, perhaps together with partial melting, all play important roles (for reviews see Garnero and McNamara, 2008; Lay and Garnero, 2004). A long standing idea, increasingly supported by seismological observations (Bolton and Masters, 2001; Deschamps et al., 2007; Ishii and Tromp, 1999; Kennett et al., 1998; Ni et al., 2002; Trampert et al., 2004) and obtained in 3-D numerical calculations (e.g. Bull et al., 2009; Deschamps and Tackley, 2008, 2009; McNamara and Zhong, 2004, 2005; Tackley, 1998, 2002), is that accumulations (“piles”) of compositionally-distinct dense material exist above the CMB and that some plumes sample this; variability in the isotopic composition of hotspots (for reviews see e.g. Hofmann, 1997, 2003; Ito and van Keken, 2007; Tackley, 2000) could thus reflect variability in the source region above the CMB. One mechanism for generating such dense piles is segregation of mid ocean ridge basalt from slabs, which has been investigated in many global numerical studies (Brandenburg and van Keken, 2007; Christensen and Hofmann, 1994; Davies, 2002; Nakagawa and Buffett, 2005; Nakagawa and Tackley, 2005a; Ogawa, 2003;
Xie and Tackley, 2004a,b). Segregated basalt could be important in generating the HIMU isotopic end member (Christensen and Hofmann, 1994; Xie and Tackley, 2004b), influence other trace element ratios such as of helium (Xie and Tackley, 2004a), and also be a repository for heat-producing trace elements (Coltice et al., 2000); therefore it could be very important in the mantle’s major and trace-element evolution. Furthermore, such dense piles would have a large effect on the dynamics and evolution of the geodynamics by their effect on the time evolution of core heat flux (Nakagawa and Tackley, 2005a, 2010) and lateral variations in CMB heat flux (Amit and Choblet, 2010; Nakagawa and Tackley, 2008), as well as the physical structure of the mantle. In global numerical models, however, it is not clear whether the physical processes by which basalt segregation can occur, are fully or properly resolved. This doubt arises not only because of limited numerical resolution and/or simplifications in the material properties, but also because the slabs in such global models are symmetric, with basalt in the centre and harzburgite on either side, in contrast to the asymmetrical stratification of actual slabs. For these reasons, detailed high-resolution calculations, preferably in 3-D and with material properties as close as possible to what is thought to be realistic, are needed, both to characterise the dynamics and thermo-chemical-phase structures that result from slab-CMB interaction, and to study the process of basalt segregation.

While there are many convection studies in which slab-like downwellings interact with the CMB, to the author’s knowledge there is only one published study of slabs that are asymmetrically compositionally stratified, which is the laboratory study of Olson and Kincaid (1991). In one of their experiments a slab analogue with two layers, one dense (representing basalt) and one buoyant (representing harzburgite) was dropped onto the hot lower thermal boundary layer with the ‘basalt’ layer on top. When the slab became warm enough it underwent Rayleigh–Taylor instabilities with the buoyant ‘harzburgite’ layer forming plumes that rose through the ‘basalt’ layer, allowing the ‘basalt’ to settle onto the hot lower boundary. After this initial rapid harzburgite escape phase, the segregated ‘basalt’ was slowly entrained by plumes.

In the present study, numerical calculations are presented that are in the spirit of Olson and Kincaid (1991), but the use of a numerical approach allows for greater realism, with physical properties such as the variation of viscosity with temperature, progressive stratification of slab composition, and the presence of phase transitions, that cannot be modelled in the laboratory. As a result, behaviour is observed that did not occur in the laboratory experiments. Subsequent sections discuss the physical model and numerical solution method, the results, and conclusions. The Appendix gives a resolution test.

2. Model and method

2.1. Physical model

The modelled domain is a 3-D spherical patch, i.e. a region of a spherical shell, in this case at the equator and containing the lower 1500 km of the mantle (i.e. 3480–4980 km radius) with an angular extent of 0.5 rad in latitude (\(\theta\)) and 0.7356 radians in longitude (\(\phi\)), which corresponds to a patch on the CMB of size 1740 by 2556 km. The top and bottom boundaries are impermeable and free-slip, with the CMB having a fixed temperature of 4000 K and the top boundary having zero heat flux. The boundaries perpendicular to the latitude (\(\theta\)) direction are reflecting and the domain is periodic in the longitude (\(\phi\)) direction. Two-dimensional cases are also performed using a spherical annulus domain, i.e. similar to the 3-D domain but only in the radius and longitude directions (Hernlund and Tackley, 2008).

For simplicity, the Boussinesq approximation is assumed, with physical properties constant except for viscosity and density. The Boussinesq approximation is reasonable for modelling the deep mantle because the adiabatic temperature gradient is relatively low due to low thermal expansivity at these high pressures. Assumed physical properties are listed in Table 1. Several properties are uncertain at deep mantle pressures and temperatures. The thermal conductivity of magnesiowüstite (Stackhouse et al., 2010; Tang and Dong, 2010) is several times that of perovskite (Keppler et al., 2008); combined values at CMB pressures have been calculated to be as high as 28 W/Km (Hofmeister, 2008) to as low as 5.6 W/Km (de Koker, 2010) depending partly on the magnitude of the radiative component; the value chosen is between these extremes. Thermal expansivity is widely thought to be around 1.0–1.2 \(\times 10^{-5}\), consistent with PREM (Dziewonski and Anderson, 1981) and several subsequent studies (e.g., Anderson et al., 1992; Chopelas and Boehler, 1992; Komabayashi et al., 2008; Tsuchiya et al., 2005).

Viscosity is assumed to vary according to an Arrhenius law:

\[
\eta(T) = \eta_{\text{ref}} \exp \left( \frac{H_{\text{act}}}{R} \left( \frac{T}{T_{\text{ref}}} - 1 \right) \right)
\]

where \(H_{\text{act}}\) is the activation enthalpy, \(R\) is the gas constant and \(T_{\text{ref}}\) is the temperature at which the viscosity is the reference viscosity \(\eta_{\text{ref}}\). The activation enthalpy is often written as an \((E + pV)\), but for simplicity and because \(V\) is low at high pressures (Ammann et al., 2008), \(H\) is here assumed to be constant. There are reasons to think that the viscosity variation is less than that predicted by diffusion creep with a constant grain size, namely that dislocation creep may be important where slabs bend at the CMB (McNamara et al., 2001) and that grain-size evolution may reduce the viscosity variation (Korenaga, 2005); so \(H\) is set to be somewhat lower than mineral physics estimates (Ammann et al., 2008; Yamazaki and Karato, 2001) at 320 kJ/mol, which gives a viscosity variation of factor 322 between the ambient mantle temperature of 2500 K and the CMB temperature of 4000 K and of factor 54,751 between the coldest part of the model slab and the CMB. However, this value is somewhat arbitrary and the influence of higher \(H_{\text{act}}\) should be tested in future. Additionally, post-perovskite is thought to have a lower viscosity than perovskite (Ammann et al., 2010) but for simplicity and due to high uncertainty in the relevant parameters, this is not considered in this initial study.

Composition, represented by a variable \(C\), is assumed to vary linearly between crust (\(C = 1\)) and the most depleted type of harzburgite possible (\(C = 0\)). Pyrolite is assumed to have a composition \(C = 0.3\), as in many of our previous studies (e.g. Nakagawa and Tackley, 2005a; Xie and Tackley, 2004a,b). Density varies linearly

Table 1

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Domain depth</td>
<td>1500 km</td>
</tr>
<tr>
<td>CMB radius</td>
<td>3480 km</td>
</tr>
<tr>
<td>Domain width: longitude</td>
<td>0.7356 radians</td>
</tr>
<tr>
<td>Domain width: latitude</td>
<td>0.5 radians</td>
</tr>
<tr>
<td>Density</td>
<td>5000 kg/m³</td>
</tr>
<tr>
<td>Compositional density contrast</td>
<td>250 kg/m³</td>
</tr>
<tr>
<td>Specific heat capacity</td>
<td>1000 KJ/K</td>
</tr>
<tr>
<td>Thermal diffusivity</td>
<td>3 \times 10^{-2} m²/s</td>
</tr>
<tr>
<td>Thermal conductivity</td>
<td>15 W/mK</td>
</tr>
<tr>
<td>Thermal expansivity</td>
<td>1.0 \times 10^{-13} K/K</td>
</tr>
<tr>
<td>Reference viscosity</td>
<td>10^{12} Pa s at 2500 K</td>
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<tr>
<td>Activation enthalpy</td>
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<tr>
<td>Post-Pv Clapeyron slope</td>
<td>7 MPa/K</td>
</tr>
<tr>
<td>Post-Pv reference temperature</td>
<td>2500 K</td>
</tr>
<tr>
<td>Post-Pv density jump</td>
<td>66.4 kJ/m³</td>
</tr>
<tr>
<td>Post-Pv reference height</td>
<td>300 km above CMB</td>
</tr>
</tbody>
</table>
with C, with a total variation of 250 kg/m³ between C = 0 and C = 1, and 225 kg/m³ between the two extreme compositions encountered in this study, C = 0.1 and C = 1. This is consistent with, or slightly lower than, the density contrast calculated from laboratory-based mineral physics measurements (Hirose et al., 2005) and early estimates (Trifune and Ringwood, 1993), although again this is uncertain, with other groups finding a smaller density contrast (Guignot and Andrault, 2004) or even a negative contrast (Ono et al., 2005).

The post-perovskite transition is included. Consistent with the Boussinesq approximation, only its density anomaly, and not latent heat, is included (Christensen and Yuen, 1985). Parameters, as listed in Table 1 are a Clapeyron slope of +7 MPa/K (Murakami et al., 2004; Oganov and Ono, 2004) and a depth of 300 km above the CMB at a temperature of 3000 K.

2.2. Initial condition

The initial condition consists of an isothermal deep mantle with pyrolitic composition (C = 0.3), a slab segment above the CMB, and a layer of dense material (nominally basalt) above the CMB. The initial mantle temperature is 2500 K. Global numerical calculations in which a dense layer develops by the segregation of subducted basalt indicate that the layer is not pure basalt (Christensen and Hofmann, 1994); therefore it is here assumed to be 80% basalt and 20% harzburgite (C = 0.8), giving it a density anomaly relative to pyrolite (C = 0.3) of 125 kg/m³. The initial thickness of the layer is either 300 km, 150 km or 0 km (i.e. nonexistent). In some cases in which a slab is not present, the layer is stratified in composition, with C varying linearly from 0.3 at its top to 1.0 at its base. This is an idealisation of the observation that in global simulations, layers that form as a result of the segregation of subducted basalt are typically compositionally stratified rather than having a sharp interface (e.g. Brandenburg and van Keken, 2007; Nakagawa and Tackley, 2005b; Nakagawa et al., 2009, 2010).

The slab is compositionally stratified, consisting of a layer of pure basalt (C = 1) underlain by a complementary layer of harzburgite that has a linear gradient in composition resulting from melting underneath a mid-ocean ridge. The mean amount of melting is assumed to be 10%, therefore the thickness of the depleted layer is 10 times the thickness of the crust, and has a composition varying linearly from 20% depletion (C = 0.1) directly under the crust to 0% depletion (C = 0.3) at the part furthest from the crust. Numerical simulations of whole mantle convection indicate that slabs thicken when they enter a region of higher viscosity such as the lower mantle (Gurnis and Hager, 1988). Therefore, it is assumed here that slabs have thickened by a factor of almost 4, with a 30 km thick crustal layer and a 300 km thick depleted layer. This is similar to the assumed thickness of slabs in Tan et al. (2002). A suitable initial thermal profile for the slab was derived by performing one-dimensional diffusion calculations starting with an error function slab profile and a step at the top of the slab. After a few tens of millions of years it was noted that the temperature profile can be approximated as a Gaussian distribution centred ~1/3 of the distance from the original top of the slab and with a half-width of \( \sqrt{2\pi t} \) where t is the time since subduction. In the calculations

![Fig. 1. Time evolution of a thermal or thermo-chemical boundary layer at the CMB for various cases and times as labelled. Plotted are isosurfaces of temperature (red) and composition (green), with a temperature also plotted on a surface of constant radius just above the CMB. The left column is for a purely thermal boundary layer. The middle column shows the case with a 150 km thick dense layer with a sharp interface at the top. In the right column are two cases with an initial compositional gradient rather than a sharp layer, either 150 km thick (top two images) or 300 km thick (lower image). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)](image-url)
presented here a half-width of 150 km is assumed, and an initial peak temperature anomaly of $-625$ K (relative to the ambient temperature).

The slab has length 1500 km and a width of 2/3 of the domain width in the $\theta$ direction (about 1200 km), therefore leaving a gap of 1/3 of the domain width for material to flow around its side (except in 2-D cases, where there can be no gap). It initially dips in the east–west direction with one side edge placed along the reflecting north boundary, and with its lowest part a few 100 km above the CMB. The initial dip is either $10^\circ$, $45^\circ$ or $80^\circ$. In the $80^\circ$ dip case, the length had to be reduced to 1350 km in order to fit inside the domain.

2.3. Numerical model

The physical problem is solved using the code StagYY (Tackley, 2008), a development of Stag3D (Tackley, 1993, 1996), which solves for instantaneous Stokes flow using a multigrid solver with velocity and pressure defined on a staggered (longitude, latitude, radius) grid and the equations approximated using finite differences, which is equivalent to the finite volume method for orthogonal geometry (Ismail-Zadeh and Tackley, 2010; Patankar, 1980). The equations are expressed in spherical polar coordinates. Temperature is represented on grid points at the centre of each volume cell, while composition is represented on tracers and for calculating buoyancy it is converted to C on the grid points using the ratio method (Tackley and King, 2003), for which approximately 10 tracers per cell are needed. Time-stepping for the $T$ field is done using the finite-volume MPDATA method (Smolarkiewicz, 1984), while tracers are advected using a Runge–Kutta method. For 3-D cases a spherical patch is used, while 2-D cases are computed in a spherical annulus, as discussed in Hernlund and Tackley (2008). The required resolution is tested in the Appendix, which finds that a grid spacing of $\approx 10$ km is needed for this physical situation. Therefore in 2-D cases, $256 \times 128$ (longitude $\times$ radius) cells are used, while in 3-D, $192 \times 256 \times 128$ (latitude $\times$ longitude $\times$ radius) cells are used. The radial grid spacing varies by a factor of 2, being smaller near to the core-mantle boundary. The number of tracer particles is 12 per cell. For the post-perovskite transition, a phase function approach is used (Christensen and Yuen, 1985; Nakagawa and Tackley, 2005b).

3. Results

3.1. Overview

In this initial study only two parameters are varied: the initial slab dip angle ($10^\circ$, $45^\circ$ or $80^\circ$) and the initial thickness of the dense layer above the CMB (0, 75 or 150 km), a total of nine parameter combinations. These cases are run in both two-dimensional (2-D) spherical annulus and three-dimensional (3-D) spherical
patch geometries, in order to determine whether 2-D simulations can give an adequate approximation of the relevant behaviour.

One goal of this study is to characterise dynamically-plausible structures to aid the interpretation of seismic results, so many ren-

Fig. 3. The interaction of a compositionally-stratified slab with an initially isochemical CMB region in three dimensions, for three different initial slab dips as in Fig. 2. Plotted are isosurfaces of composition = 0.25 (blue, showing depleted material), composition = 0.5 (green, showing basalt) and temperature = 3000 K (red semi-transparent). Times are as labelled. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)
In order to interpret slab-CMB interaction, it is first useful to understand the behaviour of the thermo-chemical boundary layer without any slab, so this is first studied in Section 3.2.

3.2. Boundary layer dynamics (no slab)

The formation of plumes from the thermal boundary layer above the CMB has been the focus of many studies so is not studied here per se; however, it is useful to establish the behaviour for the particular parameters chosen for this study, and in particular the influence of a dense layer on the dynamics.

With no dense layer (Fig. 1 left column) the thermal boundary layer is highly unstable and forms several plumes on a timescale of 50–100 Ma. When a dense layer with a sharp top is present (Fig. 1 middle column) convective instability is delayed, presumably because of the extra diffusion time needed and the reduction in available temperature anomaly, with up to 200 Ma being necessary to form plumes. If the dense layer is not sharp, as indicated by mantle convection models in which the layer develops by segregation of subducted basalt, and here consists of a gradient ranging linearly from pure basalt to the mantle composition over a specified distance, then convective instability is greatly reduced. For a gradient over 150 km it now takes over 300 Ma for plumes to develop, and then they have a larger spacing than for the no layer or sharp layer cases, while with a 300 km thick gradient, no plumes have developed even after 360 Ma.

These results show the dramatic effect of a dense layer in delaying or reducing convective instability, consistent with the stability analysis of Le Bars and Davaille (2002), particularly one containing a compositional gradient rather than a sharp change in composition. The remaining cases presented in this paper assume a sharp interface, but the effect of a compositional gradient, and the type of compositional gradient that is likely to form in the Earth, are certainly things that should be studied in the future.

3.3. Slab-CMB interaction: isochemical CMB region

Cases with no pre-existing dense layer are presented in Figs. 2 and 3 for 2-D and 3-D respectively.

When an initially almost horizontal slab (Fig. 2 left column) reaches the CMB, the harzburgite is strongly heated, giving it a low viscosity. As it is buoyant, both compositionally and now thermally, whereas the overlying basalt layer is dense, the harzburgite flows laterally and extrudes from the ends of the slab and rises in plumes. Additionally, one or more plumes may form in the slab region and penetrate through the basalt layer, removing harzburgite from beneath the basalt, as occurred in the laboratory experiments...
of Olson and Kincaid (1991). Both of these effects allow basalt to settle to the CMB. However, due to the strong activity of plumes in this case, the basalt tends to be rapidly re-entrained: only a fraction of it remains near the CMB. Thus, plumes are initially depleted in composition, but later become enriched by entraining basalt. In 3-D (Fig. 3 left column) similar dynamics are observed. Differences are that harzburgite can now extrude from the side of the slab in addition to the ends, and that plumes forming at the slab edges are three-dimensional, with a planform that is intermediate between cylindrical and linear. By the final frame (126 Ma), several cylindrical plumes have formed from the region where the slab arrived, and are entraining what is left of the basalt.

An initially almost vertical slab (Fig. 2 right column) has a tendency to rotate such that its basaltic side faces downward. This is due to the high density of basalt and the low density of harzburgite, which impart a torque to the slab. When its basaltic side reaches the CMB it is strongly heated and its basalt can easily segregate, forming a small pile above the CMB. However, in the earliest-arriving part of the slab some of the basalt is unable to separate from the harzburgite and is entrained in a plume together with harzburgite. Later on (180–216 Ma), this slab section undergoes buckling and some of this entrained basalt is seen dripping towards the CMB. In 3-D (Fig. 3 right column) similar behaviour is observed. Cylindrical plumes form away from the slab and at the side of the slab, but the largest upwelling is a hot sheet of harzburgite, with some lateral structure in the temperature field (108 Ma plot). This harzburgite plume entrains some basalt, but most of the basalt accumulates into a linear pile (180 Ma), which continues to be the base of a plume even after the harzburgite has risen.

Fig. 5. The interaction of a compositionally-stratified slab with a 75 km thick layer above the CMB in three dimensions, for three different initial slab dips as in Fig. 2. Plotted are isosurfaces of composition = 0.25 (blue, showing depleted material), composition = 0.5 (green, showing basalt) and temperature = 3000 K (red semi-transparent). Times are as labelled. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)
With an intermediate initial dip (Fig. 2 middle column), a mixture of these behaviours is observed. The earliest-arriving end of the slab exhibits harzburgite extrusion and a through-slab plume instability, while the later-arriving part of the slab rotates to a vertical and subsequently an inverted orientation. The inverted slab fragment hovers for 10s Ma a few hundred km above the CMB, but with time the harzburgite rises and most of the basalt sinks. In 3-D (Fig. 3 middle column) several plumes form around the edge of the slab, again depleted in composition. By 216 Ma there are several small piles of basalt above the CMB with plumes rising from them, as well as strips of risen harzburgite.

3.4. Slab-CMB interaction with a preexisting dense layer

The presence of a 150 km thick dense layer modifies the behaviour discussed in the previous section and generally increases the associated timescales (Figs. 4 and 5). In all cases, the slab initially pushes aside the dense layer, creating an exposed patch on the CMB. For an almost horizontal 2-D slab (Fig. 4 left column) the presence of the layer reduces the amount of lateral slab spreading and the ends of the slab are not able to get close to the CMB. While as before, harzburgite extrudes from under the slab and a plume forms in the centre of the slab, the ends of the slab warm very

![Image](image_url)

Fig. 6. The interaction of a compositionally-stratified slab with a 150 km thick layer above the CMB in three dimensions, for three different initial slab dips as in Fig. 2. Plotted are isosurfaces of composition = 0.25 (blue, showing depleted material), composition = 0.5 (green, showing basalt) and temperature = 3000 K (red semi-transparent). Times are as labelled. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)
slowly so that it takes 250–300 Ma for the basalt and harzburgite there to separate and the harzburgite to rise. By the end, the layer has returned to being fairly flat and most of the slab basalt has joined the layer. In 3-D (Fig. 5 left column) the same features are observed, again with basalt extruding from the slab's side as well as its' ends. A “harzburgite curtain” exists along the ends and side of the slab for ~10s Ma; with time this is heated and can rise in plume-like instabilities.

A steeply-dipping slab (Fig. 4 right column) again rotates basalt-side down. Due to its initial coldness and the presence of the dense layer, the basaltic crust does not come into direct contact with the CMB, and it therefore takes longer to warm the slab and separate the two layers. Not until ~180 Ma is the slab sufficiently warm for the harzburgite to rise and the basalt to sink, joining the preexisting layer. In 3-D (Fig. 5 right column), some interesting dynamics are visible along the rising part of the slab. At 144 Ma the temperature field exhibits fingering, as does the basalt sinking into the preexisting layer at 180 Ma.

An intermediately-dipping slab (Fig. 4 middle column) is also restricted in its lateral spreading by the preexisting dense layer, and again shows a mixture of behaviours of the two end member dip cases, splitting into a basalt-up section with extruding harzburgite, and a basalt-down section that slowly heats up enough for the harzburgite to rise and the basalt to fall. In 3-D, small-scale

![Graph](https://via.placeholder.com/150x150)

**Fig. 7.** Fraction of slab basalt in the lower 300 km of the mantle as a function of time for 2D (top) and 3D (bottom) cases. Cases are as labelled in the legend, in which the first number is the initial slab dip and the second number is the thickness of the dense layer above the CMB.
Convection cells are apparent in the dense layer. Two upwelling sheets develop: one from the basalt-down part and one from the basalt-down part, which takes longer to evolve.

For all initial dip angles, after a sufficient length of time (~200–300 Ma) the solution is characterised by several plumes entraining basaltic material, with strips of risen harzburgite.

Cases with a thinner, 75 km initial layer are illustrated in Fig. 6. These look quite similar to the cases with a 150 km initial layer (Fig. 5), but structures develop more rapidly. In several cases plumes are visible that have a depleted head but an enriched tail (e.g., left column 126 Ma, middle column 90 Ma). Quite often, hot and cold structures occur in close proximity (e.g., a hot plume rising next to a cold vertical slab segment in the middle column at 90 Ma). The fingering of basalt as it drops from the slab into the dense layer is clearly visible in the right column at 108 Ma.

3.5. Segregation of slab basalt

As discussed earlier, a key question in Earth's evolution is how much basalt is able to segregate at the CMB. This is quantified for the present calculations in Fig. 7, which shows the fraction of slab basalt present in the lowest 300 km, as a function of time. Note that this is only the basalt that was originally on top of the slab, not basalt that started in the dense layer above the CMB. For a completely random distribution of basalt, this fraction would be equal to the mass (volume) fraction of the lower 300 km, which is 0.146.

The general behaviour is that of a rapid increase due to slab arrival at the CMB, followed by some amount of rapid decrease, followed by a relatively stable phase. In 2-D cases the presence of an dense initial layer makes a dramatic difference: the final segregated fraction is in the range 0.6–0.8 for cases with an initial dense layer, but only 0.15–0.25 for cases without an initial layer. For 3-D cases the difference is less dramatic because the segregated fraction is higher than in 2-D for cases with no initial layer: in the range 0.25–0.45 rather than 0.15–0.25. For 3-D cases with an initial layer the final fraction is slightly lower, at 0.56–0.72. The exact thickness of the layer does not make a dramatic difference, although in both 2-D and 3-D a thicker layer results on average in slightly higher segregation.

In summary, two points stand out: (i) the presence of an pre-existing dense layer increases the fraction of basalt that is able to segregate from the slab, and (ii) there is a significant difference between 2-D and 3-D, with 3-D cases displaying greater segregation for non-layered cases and slightly lower segregation for layered cases.

4. Conclusions

In this paper, simulations of the interaction of a compositionally-stratified slab with the CMB region are presented. Contrary to the common concept of the CMB region being a “slab graveyard”, when compositional buoyancy is accounted for the slabs do not rest in peace, but rather compositionally segregate with the buoyant harzburgite rising “from the dead” and driving vigorous plumes. The main findings are as follows:

1. Compositional stratification of the slab results in a strong torque due to the relatively high density of basalt and low density of harzburgite, which tends to rotate the slab such that the basalt side faces down. Previous global convection models have either not accounted for slab compositional variations or had symmetric slabs with the crust in the middle surrounded by harzburgite on both sides; therefore this effect has not previously been appreciated or included.

2. The general sequence of slab-CMB interaction is (i) the slab warms up (ii) harzburgite rises and basalt sinks. The details and the timescale depend on several factors.

3. Three modes of basalt segregation are observed for slabs at or near the CMB. (i) Hot harzburgite extruding from the sides and edges of a basalt-up slab resting at the CMB. (ii) Hot, harzburgite-rich plumes forming at the bottom of a basalt-up slab and removing harzburgite from under the basalt slab. This was the mode observed in the laboratory experiments of Olson and Kincaid (1991), but is less important here because much harzburgite is removed by lateral flow and extrusion. (iii) Hot basalt peeling off the underside of a basalt-down slab, which in 3-D displays fingering instabilities. Furthermore, basalt–harzburgite segregation is sometimes observed in slab segments that have already been heated at the CMB and risen a few hundred km, by a folding mechanism. Which mode is dominant depends on the slab dip angle when it reaches the CMB. For intermediate dips, the slab may split into a basalt-up and a basalt-down section.

4. Plumes form at the edge of slabs, as previously observed for purely thermal slabs (Tan et al., 2002), but here it is observed that the plume heads are dominated by depleted harzburgitic material (sometimes with small amounts of entrained basalt), whereas plume tails entrain basaltic material, consistent with laboratory experiments (Olson and Kincaid, 1991).

5. Segregation of basalt depends strongly on the presence or absence of a preexisting dense layer at the CMB and by dimensionality. A preexisting dense layer greatly increases the fraction of basalt that segregates from the slab: in 3-D this fraction is in the range 0.5–0.7 with a layer present compared to 0.25–0.45 without a preexisting layer. In 2-D calculations, basalt segregation is more effective for cases with a preexisting layer but less effective for cases without a preexisting layer.

6. A range of “interesting” structures are observed in the model CMB region, which may be useful in interpreting seismic observations (e.g., Hutko et al., 2006). Strong lateral gradients in composition and temperature are quite common. Structures include plumes next to vertical slab segments, inverted slab sections perched above the CMB, harzburgite curtains, etc.

7. The presence of a stratified layer above the CMB, as obtained in global simulations in which a layer builds up by basalt segregation, strongly suppresses plume formation.

8. 2-D simulations give a good first-order guide to the dynamics obtained in fully 3-D geometry, but inherently 3-D structures are missed (plumes versus sheets, fingering) and there is a quantitative difference in the fraction of basalt segregated.

9. The gross character of thermo-chemical structures can be reproduced using quite low resolution, giving confidence in the ability of global 3-D calculations to predict structures; however, low resolution underpredicts the fraction of segregated basalt. Grid spacing of less than about 1/3 of the initial layer thickness does not make a dramatic difference: the final segregated fraction is 0.146.

Of course, these calculations are performed for one particular set of physical parameters, many of which are uncertain, so the application of these calculations to the actual Earth must be regarded as preliminary. Uncertain properties in the deep mantle include, as discussed in Section 2.1, the background viscosity, its variation with temperature (i.e., activation enthalpy), thermal conductivity (and its variation with temperature), and the density...
contrast of MORB and harzburgite. Additional rheological complexities may exist, such as dislocation creep (McNamara et al., 2001, 2002), grain-size evolution (Korenaga, 2005), and a low viscosity of post-perovskite (Ammann et al., 2010). Indeed, while post-perovskite is included in the presented calculations, its effect is not analysed here. The thickness of a slab by the time it reaches the deep mantle is another uncertainty, and may well be less than that assumed here: ideally the slab should be introduced at the surface and allowed to thicken self-consistently as it passes through viscosity steps or gradients, but this would involve much greater computational expense. In conclusion, while it is hoped that the presented results offer a useful first-order characterisation

Fig. A1. Effect of numerical resolution on structures in 2D, at times of 108 Ma (left column) and 216 Ma (right column). The physical parameters are the same for all cases: initial slab dip of 45° and initial deep layer thickness of 75 km.
of stratified slab – CMB interaction, the robustness of the observed behaviours and their scaling (e.g. of time scales and segregated fraction) with variations in physical properties must be established in future studies.

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Appendix. Resolution test

Here the influence of numerical resolution on the observed structures and on the segregation of basalt is tested. The case with an initial slab dip of 45° and initial deep layer thickness of 75 km is run in 2-D spherical annulus geometry (Hernlund and Tackley, 2008) with grids ranging from 32 × 16 (azimuthal × radial) to 512 × 256 cells, in steps of factor two. This corresponds to an approximate grid spacing near the CMB of 80, 40, 20, 10, or 5 km. The number of tracer particles is scaled in proportion to the number of grid cells with around 12 per cell, consistent with what was found to be necessary in the tests of Tackley and King (2003), giving up to 1.6 million tracers.

Fig. A1 shows that the gross structure is reproduced even with very coarse resolution, although the structures become increasingly fuzzy with lower resolution. The 512 × 256 and 256 × 128 cases look essentially identical at both times. The 128 × 64 case has identical structures at 108 Ma but by 216 Ma there are some differences in the details.

Entrainment is more sensitive to resolution, as indicated in Fig. A2, which shows the fraction of slab basalt (i.e., basalt that was originally on top of the slab) in the lower 300 km as a function of time. If slab basalt ends up randomly distributed then this fraction is 0.146. The two highest-resolution cases are almost identical, but as resolution is decreased, less basalt remains in the deep layer, which could be either because its separation from the harzburgite is not properly resolved, or because entrainment is overestimated at lower resolution, or a combination of both factors. The result is still reasonable at 128 × 64 and 64 × 32 resolution, but is completely incorrect at 32 × 16.

In summary, for the modelled physical situation, numerical convergence requires 256 × 128 grid cells corresponding to a CMB grid spacing of about 10 km. Results that have a similar visual character but with significantly underestimated basalt segregation can be obtained with lower resolution. It is likely that the required resolution depends on the thickness of the crustal layer on the slab (in this case grid spacing of about 1/3 of the initial basalt layer thickness is required) so this will have to be re-evaluated in future if thinner layers are modelled.

References
