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High Rayleigh number thermo-chemical models of a dense boundary layer in D″

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Abstract. We simulate the effects of an intrinsically dense boundary layer at the base of the mantle on the thermal structure of D″ and the dynamics of the lower mantle. Using a finite element model of thermo-chemical convection in 2-D with a Rayleigh number of 10^7, we investigate the dynamic consequences of varying the density and of increasing thermal diffusivity in the basal layer to simulate enrichment in metals. Convection may occur within a stable layer at the base of the model mantle, leading to short (400 km) wavelength temperature variations that contrast with the longer wavelength (1500 – 2000 km) variations above the dense layer. Strong small-scale convection within the layer is not observed if the layer is only marginally stable and easily deformed.

Introduction

The core-mantle boundary (CMB), which separates the silicate and oxide mantle from the iron-alloy core, is a fundamental compositional discontinuity within the Earth. Recent seismic studies have identified complexity in the structure of the lowermost several hundred kilometers of the mantle, a region referred to as D″. Complexity includes lateral variations in the thickness of D″ as seen in regional studies, lateral heterogenities within the layer that do not necessarily correlate with structure above the layer, a thin basal layer of low seismic velocity that may be caused by partial melting, and seismic anisotropy [see review by *Lay et al.,* 1998.]

These characteristics suggest that D″ is likely a region of variable composition, as well as being a thermal boundary layer. If a chemical boundary layer has persisted for any significant time at the base of the mantle, material there must be more intrisically dense than the overlying mantle by about 6% [*Hansen and Yuen*, 1988, 1989; *Sleep*, 1994]. Possible mechanisms for producing a dense layer include enrichment in iron (or other metallic phases) due to incomplete core formation, segregation of the eclogite component of subducting slabs [*Christensen and Hofmann*, 1994], partial melting and fractionation [*Garnero and Helmberger*, 1996; *Williams and Garnero*, 1996], or reactions between the core and mantle [*Knittle and Jeanloz*, 1991]. If the layer contains metal or metal alloys, it should conduct heat more readily than overlying mantle [*Manga and Jeanloz*, 1996].

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Numerical models of a dense layer at the base of the mantle show the layer piling up beneath upwellings, thinning beneath downwellings, and developing small-scale structure [*Christensen*, 1984; *Davies and Gurnis*, 1986; *Hansen and Yuen*, 1989]. Rayleigh numbers for these models range from $1 - 5 \times 10^5$. Temperature-dependent viscosity enhances small scale convection within the boundary layer [*Christensen*, 1984]. Models examining whether a layer can form by chemical reactions between the mantle and core [*Hansen and Yuen*, 1988; *Kellogg and King*, 1992; *Kellogg*, 1997] indicate that the density of the reaction products and the rate of influx across the CMB control the thickness of the resulting chemical boundary layer.

Farnetani [1997], using higher Rayleigh numbers and temperature-dependent rheology, examined the effects of a 30 – 60 km thick dense layer on the thermal structure of axisymmetric plumes. She determined that because dense material is not entrained in upwellings, the excess temperature in plume heads that reach the surface is reduced to realistic values (compared to strictly thermal models). Hence a thermo-chemical boundary layer at the CMB may account for the temperature of mantle plumes inferred from petrological models.

Numerical model

Most previously published numerical models of the dynamics of the D″ region have used relatively low values of the Rayleigh number (around 10^5). At higher Rayleigh numbers, convection is more vigorous, and complex structures can develop in D″. We have run a series of numerical models with a dense layer representing D″ and a range of Rayleigh numbers (10^5, 10^6, 10^7) and have found that models with high Rayleigh number (10^7) exhibit enhanced small scale

Table 1. Model parameters

Parameter	Definition	Value
Le (Lewis number)	κ_o/D	$10^3, 10^4$
Ra (Rayleigh number)	$\frac{\rho g \alpha_v \Delta T d^3}{\mu \kappa_0}$	10^7
B (Buoyancy number)	$\frac{\rho \alpha_v \Delta T}{\Delta \rho_c}$	$0.6, 1.0$
κ (Thermal diffusivity)	κ_0 or $\kappa_0(1+C)$	$1-2$

κ_0 is reference thermal diffusivity, D is chemical diffusivity, g is gravitational acceleration, α_v is the thermal expansion coefficient, ΔT is the temperature contrast, d is depth of the convecting layer, μ is viscosity, $\Delta\rho_c$ is the density contrast due to compositional variation.

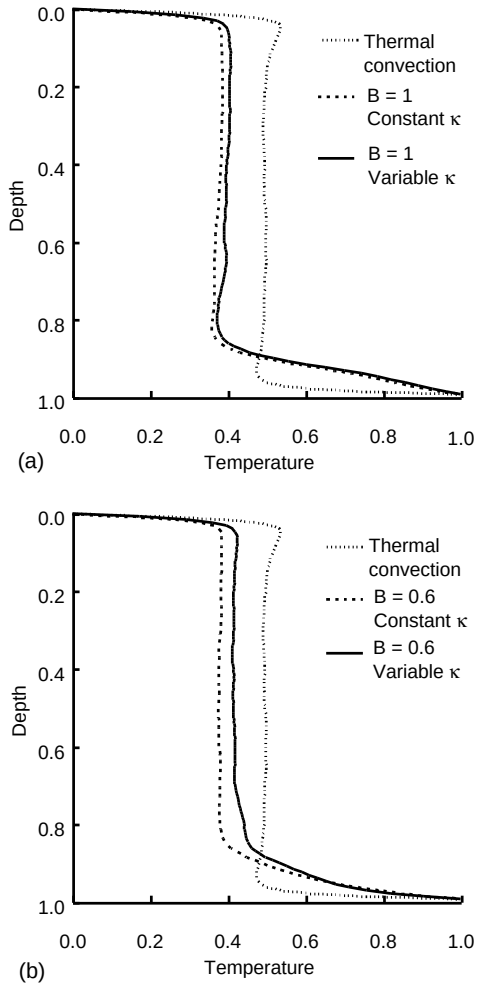

Figure 1. Laterally-averaged temperature at a dimensionless time $t = 0.008$. Dotted lines show reference case of convection with no composition. (a) $B = 1.0$ and $\mathrm{Le} = 10^4$. In (b) $B = 0.6$ and $\mathrm{Le} = 10^3$.

features within the thermo-chemical boundary layer. Due to space considerations, we present only the higher Rayleigh number models in this letter. We focus on two factors: the direct influence of intrinsic density of material in the layer, and the effect of increased thermal conductivity κ in the layer (likely if the dense layer is enriched in metals).

We use a modified version of the finite element computer code, ConMan, to solve the equations for flow of an incompressible, constant viscosity, Newtonian fluid [*King et al.*, 1990]. Changes in density are due only to thermal expansion and differences in composition. Thermal diffusivity can vary with composition (see Table 1 for model parameters). Chemical diffusion is small over the timescales in our models since the Lewis number is at least 1000; we use the method of *Lenardic and Kaula* [1993] to minimize numerical dispersion. In practice, diffusion is likely controlled by grid size.

Calculations are performed in a 5×1 box with a grid of 400×96 elements. Nodes are concentrated in the top and bottom 1/5 of the box, giving the elements in those regions an aspect ratio of 1.5, while all other elements have an aspect ratio of 1. Starting conditions include a 0.07 (equivalent to 200 km) thick compositionally distinct layer at the base of the box; we chose this thickness to resemble the average thickness of Earth's D″ layer. Initially the box has

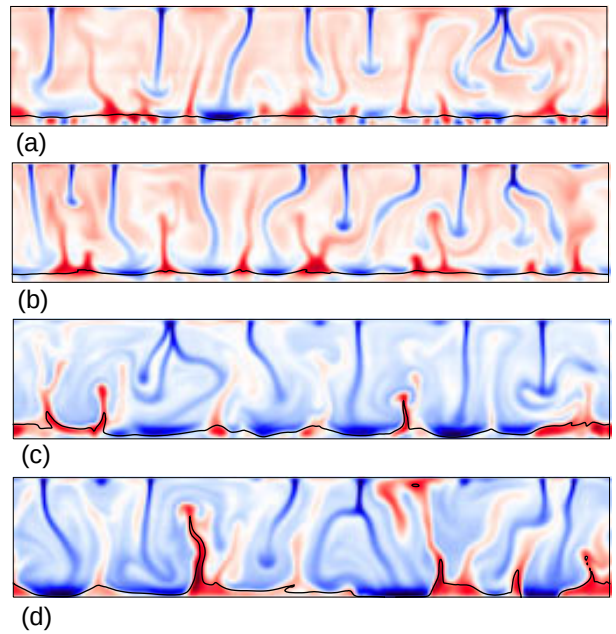

Figure 2. Residual temperature (color) after subtraction of the laterally averaged temperature profile (Fig. 1). Line shows the boundary between intrinsically dense and background material ($C = 0.5$). Dimensionless time is $t = 0.008$. (a) κ is constant, $B = 1.0$, and $\mathrm{Le} = 10^4$. (b) same parameters as (a) except κ varies with composition and is doubled in the dense boundary layer. (c) κ is constant, $B = 0.6$, and $\mathrm{Le} = 10^3$. (d) same as (c) except κ is variable.

an isothermal core ($T = 0.5$) and linear thermal boundary layers at the top and bottom of the box. Temperature is held fixed at the top ($T = 0$) and bottom ($T = 1$) of the box. Models ran for at least several overturn cycles so that the initial conditions no longer exerted a strong influence on

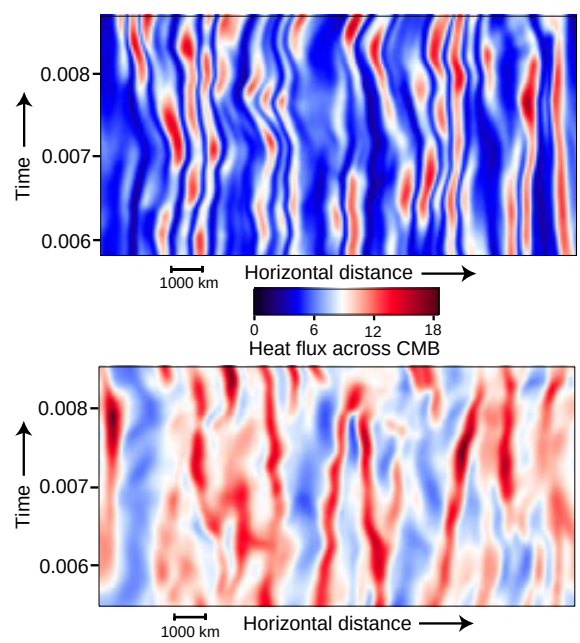

Figure 3. Time history of heat flux across the core-mantle boundary. $B = 1.0$; $\mathrm{Le} = 10^4$. Top: κ is constant. Bottom: κ is variable.

the thermal state of the model. Restricting the calculation to 2-D allowed us to perform long model runs with high grid resolution on moderate-sized computers. The sidewalls are insulating and no internal heating is included. The "dye" representing denser material does not enter or leave the box. All boundaries are stress-free.

Model results

We ran a series of models using different values of the buoyancy number, B, the ratio of thermal to chemical Rayleigh numbers (including $B = 0$, 0.5, 0.6, 1.0, 1.5). For each value of B, we ran one model with uniform thermal diffusivity, κ, and a second model in which κ varied linearly with composition (Table 1). Our functional dependence of κ was chosen to approximate the effect of adding a small amount (around 10%) of metal oxides to the silicate material that makes up the rest of the mantle [*Manga and Jeanloz*, 1996]. More iron would enhance the effects we illustrate below.

A dense layer strongly influences the style of flow. When $B > 0.5$, the dense basal layer remains distinct for at least the 10 – 12 overturn times represented by the model. Here we present two representative cases: $B = 1.0$, in which the layer is very stable, and $B = 0.6$, in which the layer survives for the duration of the model but shows extensive topography. In laterally averaged temperature profiles (Fig. 1), the thermo-chemical boundary layer resembles a thicker, lower gradient boundary layer compared to a reference model with no dense layer. Interior temperatures in the overlying mantle decrease for both $B = 1$ and 0.6, and the heat flux across the CMB is reduced.

The overall structure and topography of the boundary layer depends strongly on its density. When $B = 1$, the dense layer remains almost flat-lying (Fig. 2a and b). Upwellings cause dense material to pile up beneath them whereas downwellings are able to depress the boundary but are not strong enough to push the dense material completely aside.

The situation is different when B is reduced to 0.6. The dense layer interacts more with the overall flow due to the smaller density contrast. Downwellings push the dense material aside and upwellings create larger piles of dense material than when $B = 1$ (Fig. 2c and d). A negligible amount of dense material is entrained by upwellings during these model runs.

Differences in the internal structure of the dense layer are also produced by varying κ. This is most clear when $B = 1$; we observe small scale convection within the dense layer when κ is held constant (Fig. 2a), but not when κ is increased within the layer by a factor of two (Fig. 2b). The pattern persists for long times, as is seen by examining how the heat flow across the CMB evolves through time (Fig. 3).

For $B = 1$, where there is not much topography on the layer, it is possible to estimate a Rayleigh number for the D″ region. Taking $d = 0.07$ and $\Delta T \approx 0.6$ (Fig. 1), $\mathrm{Ra}_{\mathrm{D}''} \approx 2000$ when κ is constant, and 1000 for variable κ. Because $\mathrm{Ra}_{\mathrm{D}''}$ is only slightly supercritical for constant κ, the pattern can be resolved by this finite-element grid. Factors such as temperature-dependent viscosity that substantially increase $\mathrm{Ra}_{\mathrm{D}''}$ will require substantially finer grid resolution.

For $B = 1$ and constant κ, the small convection cells in the layer show little correlation with convection in the overlying layer (Fig. 4a and b). This suggests that fine structure at the base of the mantle may not be well correlated with structure in the overlying mantle.

The greater variation in thickness of the dense layer seen when $B = 0.6$ results in a very different thermal structure than when $B = 1$. Lateral variations in temperature are quite large as there are several large cold regions where downwellings have pushed into the hot boundary layer (Fig. 4c). Lateral variations in heat flux across the CMB also increase in amplitude due to uneven thinning of the thermo-chemical boundary layer.

When $B = 0.6$, the dense layer exhibits some internal circulation whether κ is constant or variable, possibly because the layer consists of piles of greater thickness than when $B = 1$ (increasing the value of d in $\mathrm{Ra}_{\mathrm{D}''}$). This circulation appears to be driven mostly by the convection pattern of the

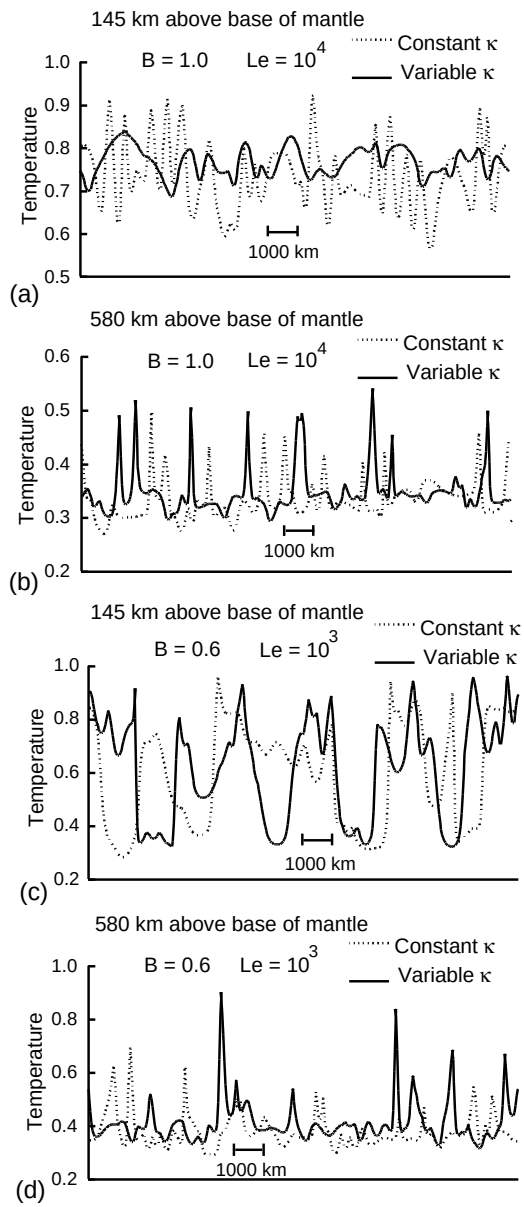

Figure 4. Horizontal temperature profiles at $t = 0.008$.

overlying layer; hot regions in the dense layer are associated with upwellings in the upper layer. Increasing κ again reduces the small scale circulation within the boundary layer and increases the temperature of upwellings (Fig. 4d).

Complexity in the thermal structure of the dense layer affects heat flux across the core-mantle boundary. All models with a dense layer show reductions in basal heat flux but with lateral variations that depend on the wavelength of structure in the layer (Fig. 3). Sporadic penetration of downwellings into the layer can lead to abrupt increases in core heat flux in regions that experience thinning of the basal layer.

Implications and Conclusions

For a chemical boundary layer at the base of the mantle to be stable through long periods of time, its intrinsic density must be high enough to prevent rapid entrainment by plumes. When the density is high enough (for instance, $B = 1$) the stable layer has low surface topography and may undergo internal convection. We can estimate $\mathrm{Ra}_{\mathrm{D}''}$ for the Earth by assuming that the temperature drop across the lowermost 250 km of the mantle is at least 800 K. Using $\kappa = 10^{-6}\mathrm{m}^2/\mathrm{s}$, $\alpha = 10^{-5}\mathrm{K}^{-1}$, and $\mu = 10^{21}\mathrm{Pa\,s}$, we obtain $\mathrm{Ra}_{\mathrm{D}''} = 7000$; certainly high enough for internal convection. However, this value is extremely sensitive to uncertainties in all the values used, especially the viscosity, which is poorly constrained in the lowermost mantle; it will vary strongly with temperature.

When the layer is only marginally stable ($B = 0.6$), its shape is irregular: large piles of material are found beneath upwellings while the layer becomes quite thin beneath downwellings. For this "lumpy" layer, a simple Rayleigh number analysis is probably not adequate; the flow implies a complex interaction between the layers.

Small scale convection in a boundary layer at the base of the mantle can create fine structure (400-500 km) that may not be correlated with long wavelength (> 1000 km) features in the overlying mantle. Without internal circulation, structure within D″ is more likely to be associated with the large-scale mantle flow. This would yield a stronger correlation between the structure in the D″ layer and in the lowermost mantle.

Because dense material in the layer may not mix freely with material in the overlying mantle, heat is "trapped" within the layer, implying higher CMB temperatures. This may result in lower viscosity and partial melting, either of which would enhance internal convection within the layer. Higher thermal diffusivity due to enrichment in metals acts to suppress internal convection in the models, but may not be sufficient to do so in the Earth's lowermost mantle. Enrichment in metals also increases the temperature of upwellings in the overlying mantle, partially counteracting the tendency of a dense basal layer to reduce temperatures in plumes.

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