The influences of composition-sand temperature-dependent rheology in thermal-chemical convection on entrainment of the D′′-layer

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Abstract

The entrainment dynamics in the D′′-layer are influenced by multitudinous factors, such as thermal and compositional buoyancy, and temperature- and composition-dependent viscosity. Here, we are focusing on the effect of compositionally dependent viscosity on the mixing dynamics of the D′′-layer, arising from the less viscous but denser D′′-material. The marker method, with one million markers, is used for portraying the fine scale features of the compositional components, D′′-layer and lower-mantle. The D′′-layer has a higher density but a lower viscosity than the ambient lower-mantle, as suggested by melting point systematics. Results from a two-dimensional finite-difference numerical model including the extended Boussinesq approximation with dissipation number $D_i = 0.3$, show that a D′′-layer, less viscous than the ambient mantle by 1.5 orders of magnitude, cannot efficiently mix with the lower-mantle, even though the buoyancy parameter is as low as $R_\rho = 0.6$. However, very small-scale schlieren structures of D′′-layer material are entrained into the lower-mantle. These small-scale lower-mantle heterogeneities have been imaged with one-dimensional wavelets in order to delineate quantitatively the multiscale features. They may offer an explanation for small-scale seismic heterogeneity inferred by seismic scattering in the lower-mantle. © 2002 Elsevier Science B.V. All rights reserved.

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1. Introduction

Almost 30 years ago, lower-mantle seismic heterogeneity close to the core mantle boundary (CMB) was detected from travel time anomalies due to the seismic phase precursor PKP (Cleary and Haddon, 1972; Cleary, 1974). Since then D′′-layer and lower-mantle heterogeneity was found on all length scales. Models of seismic wave propagation have shown, that these PKP precursors can be explained by either small-scale CMB topography undulations or by deep lower-mantle heterogeneity (e.g. Bataille and Flatte, 1988). However, recent seismological studies using PKP and PKKP precursors indicate a uniform distribution of small-scale low-amplitude scatterers throughout the mantle (Hedlin et al., 1997; Shearer et al., 1998). Moreover, the P-wave reflectivity of the D′′-layer was
explained by heterogeneities with scale lengths in the range of 10–100 km (Reasoner and Revnaugh, 1999), and recent investigations by (Cormier, 1999; Cormier, 2000) on seismic scattering further underscored the multiscale nature of the heterogeneities in the deep mantle. These observed small-scale seismic velocity perturbations can be due to small-scale compositional heterogeneity resulting from incomplete convective mantle mixing, because of long mixing time-scales for fluids having a large lateral viscosity contrast (Spence et al., 1987; Manga, 1996). Seismic scattering in the lowermost mantle is also attributed to scattering at partial melt, when the scatterers fall into the ultralow velocity zone (Garnero et al., 1993; Garnero and Helmberger, 1995; Garnero and Helmerger, 1998). Therefore, the question is, where do these small-scale compositional heterogeneities come from. In an attempt to address this question, we will study with a marker-convection model the plume driven mixing behavior of the Earth’s D′-layer (Dahm, 1934; Dahm, 1936) with the lower-mantle. It has long been suggested (Davies and Gurnis, 1986; Hansen and Yuen, 1988), that the D′-layer is chemically distinct from the overlying mantle, but its origin is still debatable. Possible mechanisms seem to be: (1) chemical reactions between iron core and silicate mantle (Knittle and Jeanloz, 1986; Song and Ahrens, 1994), (2) the breakdown of (Mg, Fe)SiO3-perovskite (Saxena et al., 1996; Mao et al., 1997), (3) the accumulation of (parts of) subducted slabs (Grand et al., 1997; van der Hilst et al., 1997) at the base of the mantle, and possibly any combination of these mechanisms, which finally would lead to the formation of an oxide-rich D′-layer (Anderson, 1998; Ruff and Anderson, 1980).

Formation of the D′-layer by the segregation of FeO from the ambient lower-mantle has been modeled by double-diffusive thermochemical convection (Naueheimer et al., 1996), and by the segregation of eclogite from deeply subducted slabs, using a marker technique for tracing the different components, within the framework of the Boussinesq approximation (Christensen and Hofmann, 1994). An additional negative compositional buoyancy equivalent to \( R_b = 1.5 \) was needed to stabilize the forming D′-layer at the CMB.

The use of markers to portray mixing processes (Olson et al., 1984; Hoffman and McKenzie, 1985) has been around for a long time and extension has been made to three-dimensional space (Schmalzl et al., 1996), where it was shown that due to both geometry of the flow and the dynamics, mixing might be less efficient than in two dimensions. Up to now, mixing processes in mantle convection have often been restricted to thermal convection, even with variable viscosity studies (Ten et al., 1997; van Keken and Ballentine, 1999). In this study, we will investigate mixing efficiency in the presence of both thermal-chemical convection and temperature- and composition-dependent viscosity.

Our intention is not to cover a large parameter space, but to draw attention to the complicated phenomenology coming along with the mixing dynamics of different mantle materials. We are presenting results from a two-component numerical model of thermal-chemical convection in two-dimensional Cartesian geometry to monitor the structural evolution of an initially stratified D′-layer. An ultrahigh resolution of ‘chemical’ markers is used to resolve the entrainment structures arising from the interaction of compositionally denser D′-layer material with lower-mantle convection, to monitor the evolution of mixing and finally to investigate the mixing efficiency from chemical buoyancy and composition-dependent rheology of the D′-layer.

The dominant mode of mantle convection today consists of plate-scale flow interacting with a strongly time-dependent mantle circulation. The apparent lag between the surface plate configuration and the lower-mantle was explained by a large viscosity increase in the lower mantle or by some layered mantle convection (Chase, 1979). Slabs subducting in the upper mantle may not be blocked temporarily by endothermic phase transition (Christensen and Yuen, 1984). This would seriously exert a dramatic effect on the flow structures and cause a triggering of lower-mantle plumes (Honda et al., 1993), like the one causing the Pacific superswell (Cazenave and Thoraval, 1994; Maruyama, 1994).

Another prominent lower-mantle upwelling, the hot plume under Africa (Ritsema et al., 1998), may be located there, because of higher mantle temperatures due to the continent’s blanketing effect, amplified by its immobility with respect to the hotspot reference frame since the opening of the Atlantic about 100 Ma ago, as suggested by the regular appearance of the seafloor magnetization (Müller et al., 1997).
Because of the manifold interactions between plates and global mantle circulation, we have not included plates or subducting slabs in our model, to avoid unnecessary complications and to focus on the dynamics in the deep mantle.

The entrainment structure modeled, here, may well describe those plumes in the deep mantle produced by various forms of focussing processes (Hansen et al., 1993), which may be responsible for the megaplumes like under the Pacific (Cazenave and Thoraval, 1994) or under Africa (Ritsema et al., 1998).

In Section 2 we give a model description of the thermal-chemical convection employed. This then is followed by a comparison between the style of plume convection near the CMB for constant and variable viscosity, in which the composition-dependent viscosity will be emphasized. We then apply the wavelet method to analyse the multiscale nature of the thermal-chemical plumes developed in the lower-mantle. Section 6 gives a summary and conclusions drawn from these simulations.

2. Thermal-chemical convection—model description

The problem to be studied is the mixing and entrainment characteristics of a dense D′-layer material with the ambient lower-mantle. Our lower-mantle model of thermochemical convection in two-dimensional Cartesian geometry is covering a depth of 2000 km. The aspect ratio is one, because of the high resolution required to resolve the fine structures presented in the following sections. We are using the finite-difference program FDCON, developed by Schmeling (Wen-berg and Schmeling, 1992), which combines a finite-difference and marker technique to solve the below mentioned partial differential equations (PDE) governing multi-component thermochemical convection. FDCON was successfully checked in benchmark tests (e.g. Blanckenbach et al., 1989; van Keken et al., 1997) and applied to several multi-component problems (e.g. Schott and Schmeling, 1998; Walzer and Hendel, 1997). Our approach, based on a finite-difference and marker technique, calls for the solution of three conservation equations for 1. mass and momentum, combined together as an elliptic partial differential equation for the stream-function $\Psi$ with either constant or variable viscosity $\eta$ and both thermally and compositionally induced buoyancy forces (Eq. (1));

2. energy, resulting in an equation for the heat transport, and including the effects of viscous and adiabatic heating (Eq. (2));

3. composition, by applying a marker approach to keep track of the high- and low-density components being advected by the convective velocity field.

The elliptic PDE for the streamfunction $\Psi$ is solved over an equidistant 121 $\times$ 121 FD-grid in the limit of $Pr \to \infty$ by the Cholesky decomposition method. The extended-Boussinesq approximation (e.g. Christensen and Yuen, 1985) is used. Its non-dimensional form is

$$
\frac{\partial^2 \Psi}{\partial z^2} + \frac{\partial^2 \Psi}{\partial x^2} + \frac{\eta(C,T,z)}{\kappa T_0} \frac{\partial^2 \Psi}{\partial x \partial z} = -R_0 \frac{\partial T}{\partial x} - R_C \frac{\partial C}{\partial x}
$$

(1)

where the viscosity $\eta = \eta(C, T, z)$ or $\eta = constant$. The equation for the heat transport becomes

$$
\frac{\partial T}{\partial t} + (\vec{v} \cdot \nabla)T = \kappa \Delta T + D_i \left( \frac{\Phi}{R_0} - v_z(T + T_0) \right)
$$

(2)

where $T$ denotes the temperature, which is non-dimensionalised by the scaling temperature $T_{scale} = 1000 K$. Eq. (2) is solved on a grid with four times higher spatial resolution (481 $\times$ 481 grid points). The surface temperature $T_0 = 0.273$ is included and the thermal diffusivity $\kappa$ is constant. $\vec{v}$ is the velocity field and $v_z$ is the vertical velocity component. $C$ is the chemical field representing a binary system consisting of D′-layer material (high density) and ambient lower-mantle (low density) substance. $\kappa$ and $z$ are the horizontal position and the depth.

In Eq. (1) the thermal and the chemical Rayleigh numbers are defined as $R_0 = \rho_0 \Delta \rho b^3/\kappa T_0$ and $R_C = \Delta p \rho b^4/\kappa T_0$, respectively, and $D_i = a g h / \kappa T_0 = 0.3$ is the dissipation number. The dissipation function $\Phi$ is defined by the relation $\Phi = 2\rho e\delta e_0$ (van den Berg and Yuen, 1997). As an equation of state we use $\rho(T, C) = \rho_0 (1 - \alpha T + C \Delta \rho/\rho_0)$, where $\rho_0$ is the reference density, $\Delta \rho$ is the density difference due to the chemical composition and $\alpha$ is the thermal expansivity. $\Delta T$ is the
temperature difference between the bottom and the top surface, \( h \) is the distance between bottom and top, respectively and \( \eta_0 = 10^{21} \text{ Pa s} \) is the scaling viscosity of the mantle, the acceleration of gravity \( g \) points in the \( z \)-direction.

FDCON is using a marker approach with a fourth-order Runge–Kutta integration in time combined with a predictor-corrector method. The markers are carrying the values \( C = 0 \) or 1, representing the different materials by their densities and rheologies, to minimize numerical diffusion. The markers are advected with the flow, and for each time-step the effective composition \( C \) is calculated from the surrounding markers at each finite difference grid point. The density and rheology is then chosen according to the actual \( C \) value (Weinberg and Schmeling, 1992; van Keken et al., 1997). The exact percentage of mantle to D″-material is given by the value of the \( C \)-field, which comes from measuring the relative fraction of the two types of markers within a local grid area. A pure mantle material is given by \( C = 0 \), while \( C = 1 \) represents an area occupied only by D″-material.

The \( C \)-field, which exists on a grid with spatial resolution \( d_x d_z \), is interpolated from the irregularly distributed markers by counting the markers within a square of dimensions \( d_x d_z \) centered at each grid point \((i, j)\). When the resolution of the grid, on which the \( C \)-field is interpolated, becomes too fine, then it can happen, that there are marker-free squares within a \( C = 1 \) domain, getting the value \( C = 0 \) by default. In this case, the interpolation produces a few singular \( C = 0 \) points within the \( C = 1 \) domain, which are purely numerical. This type of interpolation of the \( C \)-field by counting markers within grid squares works well as long as the grid spacing \( dx \) is larger than approximately \( 2 \sqrt{2} d_m \), where \( d_m \) is the average marker spacing. The \( C \)-field can therefore easily be interpolated on a \( 361 \times 361 \) grid from \( 1000 \times 1000 \) irregularly but ‘almost uniformly’ distributed markers.

3. Boundary and initial conditions

The square computational domain has free-slip boundaries at the top and bottom boundaries, including reflecting boundary conditions at the vertical side-walls. The thermal boundary conditions are isothermal top (\( T = 0 \)) and bottom (\( T = 1 \)), developing a thermal boundary layer at the CMB over which the temperature increases by \( \approx 1000 \) K. Heat flux through the side boundaries is set to zero.

Initially the model area is isothermal (\( T = 0 \)) with a hot bottom boundary (\( T = 1 \)) and a thermal perturbation in the left lower corner. Therefore, cold-looking temperatures like \( T = 0.1 \) are representing material, that is 100 K hotter than the surrounding material and the area, where \( T \geq 0.1 \) will be used to define thermal plumes and boundary layers.

The D″-layer material is initially stratified along the bottom boundary, the CMB, with a constant thickness of 200 km (Hansen and Yuen, 1988; Sidorin et al., 1999) (Fig. 1).

![Fig. 1. Initial conditions illustrated by the marker distribution with the streamlines overlaid (left panel) and the isothermal temperature field (right panel). D″-markers appear black in the left panel. Ambient lower-mantle markers are not shown.](image-url)
Table 1

<table>
<thead>
<tr>
<th>Model</th>
<th>η</th>
<th>Rρ</th>
<th>Ra</th>
<th>Dσ</th>
</tr>
</thead>
<tbody>
<tr>
<td>C0</td>
<td>Constant</td>
<td>– 0</td>
<td>10^6</td>
<td>0.3</td>
</tr>
<tr>
<td>C1</td>
<td>Constant</td>
<td>– 0.4</td>
<td>10^6</td>
<td>0.3</td>
</tr>
<tr>
<td>C2</td>
<td>Constant</td>
<td>– 0.6</td>
<td>10^6</td>
<td>0.3</td>
</tr>
<tr>
<td>C3</td>
<td>Constant</td>
<td>– 0.8</td>
<td>10^6</td>
<td>0.3</td>
</tr>
<tr>
<td>V3.1</td>
<td>Variable</td>
<td>40</td>
<td>0.4</td>
<td>10^6</td>
</tr>
<tr>
<td>V3</td>
<td>Variable</td>
<td>30</td>
<td>0.4</td>
<td>10^6</td>
</tr>
<tr>
<td>V2</td>
<td>Variable</td>
<td>30</td>
<td>0.6</td>
<td>10^6</td>
</tr>
<tr>
<td>V1</td>
<td>Variable</td>
<td>30</td>
<td>0.8</td>
<td>10^6</td>
</tr>
</tbody>
</table>

a Symbols are explained in the text.

4. Results

The runs we have conducted are based on either constant viscosity (Section 4.1) or variable viscosity (Section 4.2), which depends on composition, temperature, and depth. We have varied the buoyancy parameter $Rρ = Rρ/Ra = Δρ/(ρ0 ΔT)$ from no chemical buoyancy, $Rρ = 0$, to strongly chemically buoyant, $Rρ = 0.8$. An overview of the models is given in Table 1. Here, we want to draw the reader’s attention to the technical point, that it is very difficult to display all of the markers, because there are so many of them. We cannot see individual markers any longer because of their extreme dense spacing. In Fig. 1, left panel, the $D^\prime\prime$-markers are shown in black, resulting in a dark $D^\prime\prime$-layer, while the ambient lower-mantle markers are not at all shown.

In Fig. 2, left panel, single markers are visible in the compositional plume head (at least in a zoom-in) due to a change in marker spacing from the internal fluid deformation. In this case, it would not help markers by increasing the size of the markers. They would simply overlap each other, producing anything but a black unstructured area.

4.1. Constant viscosity

We first show how a constant viscosity plume without any chemical buoyancy, $Rρ = 0$, would behave as a reference model with other more complicated plumes to follow. We also show the development of the markers, originating in the $D^\prime\prime$-layer. This starting plume is thermally driven and is entirely composed of pristine $D^\prime\prime$-material. The material boundary between $D^\prime\prime$-layer and the ambient lower-mantle is nearly parallel to the $T = 0.1$ isotherm, in the starting plume scenario, as depicted in Fig. 2. As already stated, the $T = 0.1$ isotherm is used for defining the thermal plume.

In Fig. 3, we show the effects from a small amount of chemical buoyancy, $Rρ = 0.4$, due to the denser $D^\prime\prime$-material. The thermal plume (area in which $T ≥ 0.1$) becomes now larger than the compositional plume filled with the $D^\prime\prime$-material. The compositional buoyancy decelerates the rising plume and thermal diffusion is more effective in removing heat from the plume due to the longer time of plume evolution.

This effect becomes more prominent with a larger chemical buoyancy of $Rρ = 0.6$ (Fig. 4). In this case,
the thermal plume speeds away upward from the compositional plume, giving rise to a situation in which the thermal plume has a bigger head than that of the compositional plume upon reaching the surface.

With an additional influx of denser material at $R_{\rho} = 0.8$, hill-like structures are formed (Hansen and Yuen, 1988, 1989), since the really dense material cannot be entrained into the thermal plume any longer. This scenario of little entrainment is displayed in Fig. 5. The D″-layer now thickens, giving rise to the interesting possibility for internal convection to occur in the D″-layer, which can be clearly discerned inside the D″-layer in the right panel of Fig. 5. Hansen and Yuen, 1989 also found some evidence for such a type of internal convection inside the D″-layer but their resolution was not as dense as the one used here. This type of small-scale secondary convection cells has been suggested for the foot of the D″-layer under the Hawaiian hotspot from seismic studies (Russell et al., 1998). These constant viscosity results are shown here in order to compare with the results from a more complicated rheology involving a large viscosity contrast between the D″-layer and the lower-mantle.

4.2. Variable viscosity

We now introduce a more realistic rheological model, where the viscosity $\eta(C, T, z)$ depends
Fig. 5. A compositional buoyancy of \( R_\rho = 0.8 \) of the \( D'' \)-layer material does not allow that material to enter the thermal plume any more. However, there is little entrainment (\( R_\rho = 10^5 \), model C3).

on composition, temperature, and depth, with the denser material having a weaker rheology because of a lower melting point (Weertman, 1970; Karato, 1997). This viscosity takes the following form:

\[
\eta(C, T, z) = \eta_0 \exp \left( (\alpha a + \beta)C + (\alpha + \beta)(1 - C) \right) T + T_0 \tag{3}
\]

where \( a = 1, b = 0.3 \), and \( T_0 = 273 \), resulting in a viscosity contrast of \( \Delta \eta = \eta(C = 0, T, z)/\eta(C = 1, T, z) \approx 30 \) for \( \gamma = 0.1, \lambda = 0.3 \), respectively; with the \( D'' \)-layer being the weaker material (\( \eta(C = 1, T, z) \)) than the ambient lower-mantle (\( \eta(C = 0, T, z) \)). Almost half of the viscosity drop is due to the temperature increase in the hot thermal boundary layer and plumes, and the viscosity is increasing by a factor of 4.5 over the depth of the mantle due to increasing pressure. This range of viscosity contrast between lower-mantle and \( D'' \)-material is on the conservative side of the estimates of Yamazaki and Karato, 2001, who suggest a viscosity drop of 1–3 orders of magnitude in the \( D'' \)-layer. Nearly a quarter of a century ago, it was recognized, that a constant Newtonian viscosity is too much an oversimplification in this strongly time-dependent problem (Jones, 1977).

We then increase incrementally the strength of the chemical buoyancy from \( R_\rho = 0.4 \) to 0.6 and finally to 0.8. Small-scale secondary convection is developed ever more with an increase of \( R_\rho \), as we can see from the sequence of time-frames from Figs. 6–8 (\( R_\rho = 0.4 \)) to Fig. 9 (\( R_\rho = 0.6 \)). The latter portrays a flat \( D'' \)-layer scenario due to the localized strength of chemical buoyancy. The effect of the low-viscosity in the \( D'' \)-layer, caused by the combined efforts of thermal and compositional dependence of the rheology is to inhibit mixing in the \( D'' \)-layer by virtue of the large lateral variations in the viscosity field (Manga, 1996). Therefore, from Fig. 6 even for a modest chemical buoyancy strength of \( R_\rho = 0.4 \), very much less \( D'' \)-layer material is entrained into the lower-mantle, as compared to the isoviscous case, shown in Fig. 3.

In the case of a moderately strong chemical buoyancy (\( R_\rho = 0.4 \), Fig. 6), this dense layer can be swept aside by the strong lower-mantle flow to form lumps or hills, which can reach a height of around 500 km above the CMB, when they are hot enough. This resembles the giant plume-like structures in the lower-mantle under the Pacific Ocean and Africa (Cadet et al., 1984).

Subsequently, when they have lost sufficient amount of heat, these hills would collapse. This kind of motion in the deep lower-mantle, in which the lump is always connected to the CMB, produces extremely small-scale entrainment of the \( D'' \)-material into the lower-mantle, which leads to the production of schlieren structures above the CMB. The expression
Fig. 6. D″-layer dynamics with variable viscosity visualized by the chemical composition of the two-material system—the lower-mantle and the D″-layer (black markers)—with streamlines overlaid. A not too high compositional buoyancy of $R_\rho \approx 0.4$ allows the D″-material to rise up to 500 km above the CMB ($t = 346$ Ma). However, these D″-hills collapse, when having lost sufficient heat, producing small-scale schlieren structures due to the compositional viscosity contrast of $\Delta\eta = 30$ ($t = 366$ Ma, model V3).
Fig. 7. Thermal evolution of the initially horizontally stratified isothermal lower-mantle–D′-layer system with \( R_p = 0.4 \) and \( \Delta_T = 30 \) (model V3).
Fig. 8. Evolution of the D''-layer with a viscosity contrast of $\Delta \eta = 40$, $R_p = 0.4$ (model V3.1). Again only the markers of the D''-material are shown, not to obfuscate the tiny schlieren structures developing within $\approx 200$ Ma after an initial transient period of D''-layer internal convection.
Fig. 9. $D''$-layer internal convection is dominant at higher compositional buoyancy of $R_ρ = 0.6$ and a viscosity contrast of $Aη = 30$ (model V2). Thermal plumes starting from the $D''$-hills are entraining little $D''$ material into the ambient mantle. Composition is shown by $D''$-markers in the left, and temperature in the right panels.

'schlieren' is the one used in, e.g. schlieren photography, a common technique to visualize flow patterns in experimental fluid dynamics (van Dyke, 1982). We will analyze these schlieren structures with wavelets in Section 5. A wavelet analysis of a whole time series would lie beyond the scope of this paper, where we analyze two representative snapshots, to illustrate typical multiscale features of the evolved structures. With increasing value of $R_ρ$ in the $D''$-layer of up to $R_ρ = 0.6$ (Fig. 9), the dense $D''$-layer becomes more and more stably stratified with thermal plumes issuing from the top of the hill, but entraining very little $D''$-material (Figs. 8–10). This scenario of large values of $R_ρ$ has already been studied by Hansen and Yuen (1989), Hansen and Yuen (1990) and Tackley (1998b).

5. Analysis of the schlieren structure using wavelets

The structures in thermal-chemical convection have a distinct multiscale character because of the differences in the scales of the chemical and thermal forcings and in the thermal and chemical viscosity gradients. Wavelets represent a recently developed tool in mathematics, which allows one to analyze multiscale structures in a readily understandable format (Mallat, 1998). These schlieren or tendril-like structures have been analyzed by interpolating a continuous compositional field $C$ either on a $121 \times 121$ grid or on a $361 \times 361$ grid from $1000 \times 1000$ markers, thus yielding a spatial resolution of 16.5 km or 5.5 km, respectively. These continuous $C$-fields are
Fig. 10. A high compositional buoyancy of $R_\rho = 0.8$ is causing a flat $D''$-layer ($\Delta\rho = 30$, model V1). The layer internal convection cells have aspect ratios between 1.4 and 2 with an average of 1.6. Very little $D''$-material is entrained into the ambient mantle. Composition is shown by $D''$-markers in the left, and temperature in the right panels.

displayed in Figs. 11 and 12, they have been taken from the last time-steps in Figs. 6 and 8. We are analyzing two different, however typical, schlieren structures at two different spatial resolutions in order to demonstrate the sensitivity of the analysis to spatial resolution.

First, we will focus on the high resolution grid (Fig. 12). For extracting the relevant scale information from the grid, a suitable way is to transform one-dimensional spatial profiles, using both Fourier and wavelet methods. The mixing schlieren structure shown in Fig. 12 is now analyzed along the nine horizontal profiles X1 to X9. Analysis was done along the horizontal and vertical profiles, however, the results are the same for both sets of profiles. Therefore, we are focusing on the horizontal profiles only.

Due to computational efficiency, all profiles were extended by zero leading to 512 intervals with a spacing of 5.5 km (Fig. 13). This particular spacing allows a minimum resolvable wavelength of 11 km, which is comparable to the length-scale of heterogeneities, as observed by scattered waves in PKIKP/PKP studies (Cormier, 2000). The maximum wavelength is 5632 km corresponding to twice the extended profile length. Before transforming the profiles, a linear trend was removed for avoiding aliasing effects. The horizontal profiles are located in depths ranging from 600 km in the lower-mantle (profile X1) down to 1900 km near the CMB (profile X9). The normalized Fourier amplitude spectra are shown in Fig. 14.

Obviously, the spectral energy is transferred from the short wavelengths in profiles crossing the top of
Fig. 11. Chemical field of the last time-step shown in Fig. 6 interpolated on a 121 × 121 grid, yielding a spatial resolution of 16.5 km. The locations of the examined horizontal profiles across the compositional schlieren structure are indicated by lines.

the mixing structure (profiles X2 and X3) to longer wavelengths near the CMB (profile X9). The shortest wavelength is associated with the entrainment of the D"-material.

For multiscale features, such as shown in the entrainment process, a wavelet analysis is a more suitable tool for analyzing the spatial profiles. Fourier transformation cannot identify precisely the source of the energy, it can only determine the sum of the power, while losing the phase information needed for locating the position of the heterogeneities. Additionally, the advantage of a wavelet analysis as compared to a windowed Fourier transform comes from its being scale-independent, because wavelets with short
windows are used for short wavelengths and long windows for long wavelengths. Hence, there are no aliasing effects due to high and low frequency contributions. We will take again one-dimensional profiles and determine the dominant modes of variability and how these modes would change along profile (Fig. 13). This technique has been used by Simons and Hager (1997) to examine post-glacial rebound. We have used the continuous wavelet transform (CWT) (Daubechies, 1992) and a one-dimensional Morlet wavelet (Goupillaud et al., 1984) for analyzing the 9 profiles shown in Fig. 11 and the 18 profiles shown in Fig. 12, respectively. Generally, a CWT can be written like

$$W\psi(s, \chi) = \int w(x)\psi_{s, \chi}(x) \, dx,$$

where \(\psi_{s, \chi}(x)\) represents the wavelet \(\psi_{s, \chi}(x) = (1/\sqrt{s})\psi((x - \chi)/s)\) \((s > 0, \chi \in \mathbb{R})\). A set of wavelets \(\psi_{s, \chi}(s)\) is created from a so-called mother wavelet \(\psi_{0}\) by shifting and scaling. The shifting parameter \(\chi\) is responsible for the location, and \(s\) is the scaling parameter, stretching \((s > 1)\) or compressing \((s < 1)\) the mother wavelet. We have chosen a complex Morlet wavelet (Morlet et al., 1982) for the analysis to minimize the space–wavenumber uncertainty of \(\Delta k \Delta \chi \geq 1/(4\pi)\). Here, the scaling parameter \(s\) can be regarded as a wavelength, although for most other wavelets, \(s\) has a more general meaning and is called ‘scale’. This kind of Morlet wavelet has been used recently in analyzing time-series in mantle convection (Vícey and Matyska, 2001). A complex Morlet wavelet is a plane wave modulated by a Gaussian function and takes the form

$$\psi_{s, \chi}(x) = \pi^{-1/4}(s)^{-1/2}e^{-2(x^2/(s-\chi)^2) - (x-\chi)^2/2s}$$

(4)
Fig. 13. Horizontal profiles of the chemical field. Their location is shown in Fig. 12.
Fig. 14. Fourier amplitude spectra of the nine horizontal profiles, for location see Fig. 12. Each spectrum is normalized to its maximum. The shaded lines indicate how the energy is moving from short to longer wavelength. The profiles starting at the top of the mixing structure in 600 km depth (top) down to the CMB (bottom).

Fig. 15. The nine selected horizontal profiles of Fig. 13 were analyzed using a continuous wavelet transform with a Morlet wavelet of length six. Each of the nine panels is divided into four diagrams, showing in the upper left—the wavelet-scalogram; upper right—the normalized Fourier amplitude spectrum; lower left—the analyzed profile; lower right—the real part of the Morlet wavelet. The wavelet-scalogram shows the color-coded space–wavelength distribution of the analyzed profile. Red colors indicate high-amplitudes, blue colors indicate low-amplitudes, values below 15% of the maximum are left white. The color-coded plots allow to identify both the wavelength of the individual signal as well as its location in the spatial profile, since the spatial and wavelength axes of the original profile, the Fourier spectrum and the wavelet transform are identical, respectively. The upper left panel is representing the wavelet transform of a single schlieren structure of thickness 5.5 km, here, the advantages of the wavelet transform become obvious, since the Fourier transform is not able to detect neither the wavelength nor the location of the signal. The upper three panels crossing the top of the schlieren structure show wavelengths from 10 to 40 km on the one hand, and from 200 to 400 km on the other. The middle three panels show wavelengths ranging from 100 to 700 km. Finally, the lower three panels indicate wavelengths around 1000 km representing the thickness of the base of the evolving D' structure. Thus, we identify three different levels of schlieren thickness, 6–20 km at the top, 50–350 km in the middle and round 500 km at the base of the model.
An additional parameter $l$ was introduced to allow for an arbitrary shift of the wavelet transform resolution in favor of spatial or wavenumber resolution for a fixed scale $s$ without changing the central wavenumber. We have determined $l$, the length of the wavelet, by the spatial and wavenumber resolution, thus, $l$ represents the number of oscillations of the wavelet. From the uncertainty principle, the greater the number of oscillations, the lower would be the spatial resolution and vice versa. The sampling in space and wavenumber is then determined by

$$
\Delta \chi = \frac{l}{\sqrt{2}}, \quad \Delta k = \frac{\sqrt{2}}{4\pi^2 l}, \quad \Delta s = \frac{\sqrt{2}}{4\pi^2 l}
$$

(5)
Fig. 16. The nine selected horizontal profiles of Fig. 11 were analyzed using a continuous wavelet transform with a Morlet wavelet of length six. Grouping of the panels is analog to that in Fig. 15, where the panels are explained in the figure caption. The upper left panel is representing the wavelet transform of a single schlieren structure of thickness 16.5 km. The upper three panels crossing the top of the schlieren structure show a maximum amplitude for wavelengths around 100 km, with a significant contribution for wavelengths down to some 10 km. The middle three panels show a maximum amplitude for wavelengths around 1000 km, with a significant contribution for wavelengths down to 100 km. Finally, the lower three panels indicate wavelengths around 1000 km representing the thickness of the base of the evolving D''-structure. The lower right panel indicating an amplitude shift towards shorter wavelength. Thus, we identify three different levels of schlieren thickness, 10-50 km at the top, 50-500 km in the middle and round 500 km at the base of the model.
By inspecting at the third equation in Eq. (5), we can see that a logarithmic equidistant sampling in $\chi$ is appropriate. For maintaining a balance between the spatial and the wavenumber resolution, a length of $l = 6$ was chosen. A linear fit was again removed from the profiles and each profile was then operated on by the Morlet wavelet. The numerical implementation of the CWT is a discrete convolution between the spatial profile and the discretized wavelet at all scales. For interpretation, the wavelet transform was interpolated in the space–wavenumber domain and the amplitudes were color-coded. Figs. 15 and 16 present the wavelet-scalograms of the nine respective horizontal profiles (Figs. 11 and 12) together with the spatial profile, its Fourier spectrum and the real part of the Morlet wavelet used. The L2-normalized wavelet-scalogram in the upper left box of each panel of Figs. 15 and 16 reveal clearly the high-amplitudes in red colors and the low-amplitudes in blue colors. A cut-off at 15% of the maximum is introduced for suppressing the lowest amplitudes in order to enhance the clarity.

Three different levels of tendril wavelength/thickness can be identified in both schlieren structures (Figs. 15 and 16): the upper three panels contain high-amplitudes for wavelengths between 11 and 40 km at 5.5 km resolution (Fig. 15, $361 \times 361$ grid, corresponding profiles $X1$ to $X3$ in Fig. 12) and wavelengths between some 10 and 100 km at 16.5 km resolution (Fig. 16, $121 \times 121$ grid, corresponding profiles in Fig. 11). Panels in the middle indicate wavelengths between 100 and 700 km at 5.5 km resolution (Fig. 15, $361 \times 361$ grid, corresponding profiles $X4$ to $X6$ in Fig. 12) and wavelengths between 100 and 1000 km at 16.5 km resolution (Fig. 16, $121 \times 121$ grid, corresponding profiles in Fig. 11). The lower three panels show highest values at wavelengths of about 1000 km on both grids (Figs. 15 and 16).

Thus, the corresponding schlieren thickness is 5–20 km at the top of the mixing structure, 50–500 km in the middle, and 500 km at the CMB. This result remains the same for both schlieren structures and holds for both spatial resolutions examined. Such entrainment pattern typically evolve in thermochemical convection, when a large viscosity difference between the fluids is included. It also confirms the usefulness of the wavelet analysis as a tool for examining and comparing the characteristics of multiscale structures at different spatial resolution. We note especially that the small-scale schlieren at the top of the mixing structure may explain the existence of small-scale scatterers, found in seismic wave inversions (Freybourger et al., 1999; Cormier, 2000).

6. Conclusions and discussion

The purpose of our work on compositionally dependent rheology in thermal-chemical convection is to draw attention to the complicated $D''$-layer entrainment structures most likely existing in the lower-mantle, which have the potential of explaining the observed seismic scattering. Here, we are not concerned with subduction and the overall mantle mixing processed (e.g. Gurnis, 1986a; Olson et al., 1984; Christensen and Hofmann, 1994). The results of our numerical thermal-compositional convection model show, that a low viscous $D''$-layer with a rather small density increased of 5% may not be entrained into thermal plumes starting from the $D''$-layer. A similar behavior has been found for multi-layer Rayleigh–Taylor instabilities occurring in magmatic diapirs (Cruden et al., 1995). However, the partially entrained $D''$-layer material can form distinct lumps, which do not have to have a hill-like shape with a smooth surface (Tackley, 1998a), but can have a complex tree- or polyp-like structure. Similar complex structures have been modeled by Hansen and Yuen (2000), however, their model could not resolve the small-scale structure of branches or tentacles reaching out into the lower-mantle (Fig. 12). The heterogeneity is developing the shape of a large ‘blob’ connected to long thin tendrils, which lengthen exponentially with time, while the ‘blob’ deforms much slower (Gurnis, 1986b). Similar ‘blobs’ may, therefore, explain some aspects of heterogeneity in the Earth’s mantle (Becker et al., 1999). For these tiny schlieren structures we find scaling diameters in the order of a few to 10 km, which is too small to be resolved in numerical models of double-diffusive thermal-chemical convection (Hansen and Yuen, 2000). The double-diffusive convection approach also inhibits the development of small-scale mixing (Montague and Kellogg, 2000). Schlieren structures of diameters down to about 5 km are robust features in our 2000 km $\times$ 2000 km large model and subsequent analysis, when 1000 $\times$ 1000 markers are used, because a 5 km thick ‘tentacle’
is defined by about three markers along its diameter. Additional schlieren structures with even smaller diameters could be made visible by an increasing number of markers, while already detected structures would become smoother, but would not disappear.

We suggest, that these tiny schlieren structures can explain the recently proposed uniform (Hedlin et al., 1997) or slightly depth dependent (Shearer et al., 1998; Cormier, 2000) distribution of small-scale low-amplitude scatterers throughout the mantle with typical scale-lengths around 10 km. Due to thermal diffusion pronounced small-scale thermal perturbations cannot survive on the long time-scale our models are covering, but seismic velocity perturbations on length-scales of 200–1000 km may be of thermal origin (Fig. 7).

The observed ‘non-decaying’ power spectrum of scattered seismic energy attributed to heterogeneity significantly departs from that one expected from thermal variations in a convecting mantle. The entrainment of small-scale (10–100 km) schlieren structures is a likely explanation for such a ‘non-decaying’ power spectrum (Cormier, 2000).

A maximum of about 40% of the initially strati-

fied D′′-layer material can be ‘mixed’ into the am-
bient lower-mantle within a model time of 475 Ma
(Fig. 6), if we are counting the \( C = 1 \) markers (rep-
resenting the D′′-material) having a depth shallower
than 500 km above the CMB. However, most of the
D′′-material is forming into large lumps, which are all
the time staying close to the CMB. We, therefore,
 conclude, that these lumps can still serve today as a dis-
tinct chemical reservoir in the Earth’s mantle, similar
to the deep-mantle blobs (Becker et al., 1999).

While the small-scale schlieren cause seismic scat-
tering (Cormier, 2000), the bulk of the D′-layer shows
a strong longer-wavelength topographical undulation,
which is reflected by the short-length scale horizontal
variations in the topography, due to a P-wave reflec-
tor attributed to the top portion of the D′-layer. Such
variations of the depth of the D′-reflector between 150
and 200 km have been found beneath the southwestern
Pacific (Yamada and Nakashishi, 1998) and northern
Siberia (Freybourger et al., 1999). Under northern
Siberia PdP travel times have also been explained with
a 7 km thick 3% low velocity lamella lying approx-
imately 300 km above the CMB (Freybourger et al.,
1999).

Models of mantle mixing should principally be studied in three dimensions (Ferrachat and Ricard, 1998), because it is difficult to scale the mixing behavior from 2D to 3D, and mixing in 2D is more efficient than in 3D (Schmahl et al., 1996). However, the need of very high spatial resolution and many markers to track the materials with high accuracy over long time spans is not easily achievable in 3D today. Computationally faster 2D models of thermal-chemical convection remain still a versatile tool to study basic mixing properties.

For the choice \( \text{Di} = 0 \) (incompressible convection) an isothermal mantle is the only reasonable ini-
tial condition, that is gravitationally stable. For the
choice \( \text{Di} > 0 \) (‘compressible’ convection) all initial
conditions between an isothermal mantle and an adi-
abatic temperature gradient are gravitationally stable.
While the choice of an adiabatic temperature gradi-
ent is essential from the viewpoint of thermodynam-
ics, we have chosen the isothermal initial condition to
make the different results easier to compare. We are
therefore overestimating the thermal buoyancy forces
for \( \text{Di} > 0 \). However, preliminary results for starting
with an adiabatic temperature gradient show, that even
very little additional compositional buoyancy of the
D′-layer, as low as \( R_p \approx 0.2 \), are enough for stabiliz-
ing the D′-layer at the CMB. This is in full agreement
with the results of Tackley (1998b).

Values of \( R_p \) greater than one are typically needed
to stabilize the D′-layer at the CMB when the Boussi-
nesq approximation is used together with constant ma-
terial properties, such as the thermal expansivity and
viscosity (Christensen and Hofmann, 1994; Davaille,
approximation is, therefore, not appropriate at all for
assessing the stability of the D′-layer.

We have not considered the additional stirring of
the D′-layer by other processes such as by subduct-
ing slabs, because recent numerical models show, that
cold dense downwellings sinking into the D′-layer
do not necessarily trigger instability (thermochemical
plumes) in their surrounding, by either sweeping the
D′-layer aside or by increasing the temperature gra-
dient, but may lead to the formation of highly compli-
cated structures of layered thermochemical convection
(Hansen, 2000). Moreover, subducting slabs may not
reach the CMB, but hover in the mid-lower-mantle,
due to the decreasing thermal expansivity with in-
creasing pressure (Chopelas and Boehler, 1992; Kessoon et al., 1998; Kaneshima and Helmlrich, 1999). However, this picture may change from slab to slab (Cizkova et al., 1998) because of the rheological dependence on the subducting velocity (Karato et al., 2001). Such additional complications are beyond this study, where we are focusing on the style of entrainment of D″-material into the lower-mantle. Once the D″-material is entrained by the plumes, it will certainly be further mixed into the mantle by fluid dynamical processes stirring the mantle.

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