Stability of a chemically layered upper mantle

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ABSTRACT

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The possibility that the upper mantle at depths less than 670 km is chemically as well as mineralogically layered has been extensively discussed. One idea posits that sublithospheric upper mantle (d < 400 km) is dominantly harzburgitic and of low intrinsic density compared with majoritic and clinopyroxene-rich piclogite which occupies the seismic transition region at depths between 400-670 km. The gravitational stability of the 'harzburgite over piclogite' arrangement (light above heavy) when heated from below is investigated here in order to better understand the dynamics of mixing. The calculations neglect the effects of plates, compressibility, viscous dissipation, phase change and radiogenic heating and focus on the role played by $\Delta \rho / \rho_0$, the intrinsic density difference between the layers during mixing at fixed Rayleigh number. The dimensionless parameters of this problem include the thermal Rayleigh number based on the heat flux q_0 into the basal piclogitic layers ($Rq = \alpha gq_0 d^4/k \kappa \nu$), the ratio of chemical to thermal buoyancy $R\rho = (\Delta \rho / \rho_0)k/\alpha q_0 d$, and the thickness ratio of the two layers Δ . Here α , g, d, κ , ν , $\Delta \rho$, ρ_0 represent the expansitivity, gravity, total depth, thermal diffusivity, thermal conductivity, kinematic viscosity, isothermal difference in density between the two layers (i.e. the intrinsic density difference) and density of the piclogitic bottom layer, respectively. A constant-viscosity Newtonian rheology is assumed for the sublithospheric upper mantle between 100-670 km.

Three measures of the extent and thoroughness of mixing are used to quantify mixing; these include the variance of the compositional field, the two-point spatial correlation function for composition and the average composition within each layer. The spatial correlation enables one to define a dominant length scale characteristic of the size of the chemical anomalies (L^*). The adimensional variance, sometimes called the mixing intensity, may be used to define a mixing time. Simulations at fixed Rq but with $\Delta \rho / \rho_0 = 0$, 2, 4, 8% have been carried out for periods of time equivalent to the age of the Earth. The critical $R\rho$ that separates well-mixed states from poorly mixed ones is $R\rho \approx 1/5$ for $Rq = 2 \times 10^5$. For nominal upper-mantle parameters this implies a critical intrinsic density difference $\Delta \rho / \rho_0 \approx 3\%$. The style of mixing is grossly different depending on whether $\Delta \rho / \rho_0$ is less than, or greater than, the critical value. Plume penetration with rapid changes in the average size of chemical heterogeneities is the dominant mechanism at low $\Delta \rho / \rho_0$ whereas for high $\Delta \rho / \rho_0$, viscous entrainment and the stretching of tendrils along the layer interface is the dominant mixing style. For density ratios near the critical value, the fraction of fertile (easily fused) periodite within the dominantly harzburgitic upper mantle above the top of the transition region varies quasiperiodically with period ≈ 0.6 Ga, roughly equal to the supercontinent cycle time. Intermittent periods of increased lower-layer transport across the top of the transition zone may correlate with spikes in the volumetric rate of magma generation due to decompression melting of ascending fertile periodite.

Introduction

The present chemical and mineralogical constitution of the Earth's mantle and its evolution throughout the past 4.5 Ga is a fundamental geodynamic issue. The problem is a complex one because the initial conditions prevailing at the time of earth accretion are poorly known and available constraints from petrology, mineral physics, isotope geochemistry and seismology are not sufficiently precise at present to support a unique model. In particular, it is not known whether convection in the Earth's mantle occurs in cells that extend throughout the entire depth of the mantle or if the upper and lower mantle convect in independent layers or even if the up-

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per mantle itself is characterized by layered convection. Despite uncertainty, it is obvious that the mantle is heterogeneous and that differences in density due to bulk composition, phase transitions and temperature are important in determining the circulation and mixing evolution within the mantle and hence the dynamics and interpretation of basalt geochemistry (Zindler and Hart, 1986; Allegre, 1987; Silver et al., 1988; Anderson, 1989; Galer et al., 1989; Ohtani et al., 1989; Galer and Goldstein, 1991).

The possibility that the upper mantle (d < 670km) is chemically as well as mineralogically zoned has been discussed in the literature. For example, Ohtani (1985) and Ohtani et al. (1989) have argued for an upper mantle composed of two layers -an upper olivine-rich one and lower garnet-rich one. In this model, the 400 and 670 km discontinuities represent chemical as well as phase transition boundaries. Anderson, in a series of papers (e.g. Anderson and Bass, 1984, 1986; Anderson, 1982, 1987, 1989) has argued that low-density harzburgite (olivine plus orthopyroxene) dominates the shallow (d < 400 km) part of the upper mantle, whereas a denser Al₂O₃-rich piclogite (clinopyroxene + garnet_{ss} + γ , β -spinel) makes up the transition region at depths between 400 and 670 km. It has been speculated that harzburgitic upper mantle, dominated by magnesium-rich olivine (Fo₈₇₋₉₂) and low-calcium orthorhombic pyroxene with $\approx 2-5\%$ wt. Al₂O₃, represents the residue after extraction of mid ocean ridge basalt (MORB) and perhaps komatiitic melt throughout geologic history. Mineralogical evidence for the existence of both eclogites and garnet peridotites at depths approaching the transition zone has recently been found (Sautter et al., 1991) although mineral modes and rock proportions cannot be accurately based on the limited samples available. The propensity for garden-variety alkalic basalts found on every continent and at many intraplate (hot spot) oceanic island basalt (OIB) sites to transport major element-depleted ultramafic rocks (e.g. peridotites, harzburgites, dunites) from depths of order 50 to 100 km is well known and consistent with upper mantle stratification. Alternatively, or additionally, olivine flotation in a Hadean terrestrial magma ocean may have been an important early differentiation process giving rise to a harzburgitic upper mantle at depths less than 400 km (Agee and Walker, 1988), although this issue is controversial (Ringwood, 1989, 1990; Tonks and Melosh, 1990). A key question within the framework of the 'harzburgite above piclogite' or 'light above heavy' stratified upper mantle is the stability of the arrangement with respect to heating from below. Obviously, if the difference in compositional buoyancy between the layers is small, heating of the lower layer leads to rapid mixing of the initially distinct reservoirs by the action of normal and shear strain induced by convective stresses. A related question then becomes the rate of mixing between the layers and especially the evolution of the size spectrum of compositional heterogeneities as a function of the initial density difference between the layers $(\Delta \rho / \rho_0)$ and the heat flux (q_0) into the compositionally denser bottom layer. In order to investigate this problem, we have assumed that the boundary between the upper and lower mantle ($d \approx 670$ km) is open with respect to heat but closed with respect to mass exchange. This enables us to focus specifically on the question of the stability of a chemically stratified upper mantle when heated from below.

Previous work on the problem of convective mixing within the mantle has been carried out by a number of workers in the last decade (e.g. Richter and McKenzie, 1981; Davies, 1982; Christensen and Yuen, 1984; Olson et al., 1984; Gurnis, 1986; Allegre and Turcotte, 1986; Gurnis and Davies, 1986a, b; Hoffman and McKenzie, 1986; Kellogg and Turcotte, 1987; Spence et al., 1988; Christensen, 1989; Davies, 1990; Kellogg and Stewart, 1991; Machetel and Weber, 1991; Olson and Kincaid, 1991). Olson (1984) performed an interesting set of laboratory experiments in which a two-layer system with an intrinsic (isothermal) density difference was heated from below. He found that the mixing time defined by

$$t_{\text{mixing}} \approx \left\{ \frac{1}{\Delta \rho} \left[\frac{\mathrm{d}(\Delta \rho)}{\mathrm{d}t} \right] \right\}^{-1}$$
 (1)

was a function of $\Delta \rho / \rho_0$ at fixed basal heat flux and fluid properties. Convective mixing exhibited in his experiments was driven by viscous stresses acting along the layer boundary. Mixing occurred through entrainment of convective eddies from one reservoir into the other rather than through the mechanism of freely buoyant plume penetration through the interface. His experimental results suggest that if the density jump at 670 km is due to compositional change, then significant heterogeneity on the scale of 100-1000s of kilometers will persist even after several Ga. More recently, Kellogg (1991) has investigated the interaction of thermal plumes with a compositional boundary at 670 km using a finite element model of convection in a spherical axisymmetric shell. She found that when the parameter $B \approx \Delta \rho / \rho_0$ $\alpha \Delta T < 1$, plumes readily cross the chemical boundary, whereas for B > 1, flow in the upper laver is shear coupled to the flow in the lower layer (i.e., two-layer convection prevails). For B ≈ 1 the coupling is more complex and significant mass exchange occurs across the compositional boundary although plumes per se do not cross into the upper layer. Machetel and Weber (1991) studied the role of the endothermic phase transition at 670 km (spinel \rightarrow perovskite + MgO) on the style and mechanism of convective mixing within the mantle. For a value of the Clapeyron slope appropriate for Earth, they observed intermittent mixing between the upper and lower mantle. They suggest that intermittent mixing offers a way to reconcile conflicting geophysical and geochemical evidence for both whole-mantle and two-layer convection.

In this work, we report on numerical experiments which isolate the role of the ratio of chemical to thermal buoyancy on the mixing of an initially two-layer system (light above dense) when heated from below. We emphasize that the problem studied is a simplified model of reality. The calculations ignore three-dimensional effects, the role of compressibility, radiogenic heating, viscous dissipation, phase change, and the temperature, composition and pressure-dependence of viscosity. Given the assumptions and fixing the size of computational domain, dimensional analysis shows that there are two parameters that



Fig. 1. Schematic cross-section of a two-layer upper mantle. Below the lithospheric thermal boundary-layer lid, a 300 km thick harzburgitic region with mean density $\rho_0 - \Delta \rho$ is present. The transition region, at depths between 400–650 km is made up of piclogite, a fertile garnet (majorite)- bearing lithology consisting of α , β -spinel, aluminium-rich orthopyroxene, clinopyroxene and complex garnet solid solution. The gravitational stability of the stratified system pictured in the figure with respect to heating from below (q_0 is the imposed basal heat flux) is investigated in this study.

control the nature of circulation and mixing evolution. These include the Rayleigh number, (Rq)a measure of the ratio of thermal buoyancy to viscous forces, and the buoyancy number, $R\rho$ which is proportional to $\Delta \rho / \rho_0$ where $\Delta \rho$ is the isothermal difference in density between the lower and upper layer and ρ_0 is the density of the lower layer. The main goal of this study is to investigate the dynamical evolution of an initially layered system (Fig. 1) as a function of $\Delta \rho / \rho_0$ for Rayleigh numbers typical of the upper mantle. In order to quantify the mixing evolution, attention is focused on the statistics of mixing using measures previously exploited to quantify magma mixing (Oldenburg et al., 1989; 1990). The evolution of the variance (second moment of the compositional field) and L^* , an adimensional length scale based on the correlation length of compositional anomalies (integral of the two-point spatial correlation function) are especially useful measures of mixing; their dependence on $\Delta \rho / \rho_0$ is, therefore, investigated.

The plan of this paper is as follows. In the next section, the conservation equations, parameters, boundary and initial conditions, computational domain and numerical methods are described. These relations are well known and the emphasis is on brevity. In the following section, the results of the simulations are presented emphasizing the mixing evolution and its dependence upon $\Delta \rho / \rho_0$. Finally, in the last section, we summarize and speculate on the significance of the results with respect to mixing within the mantle.

2. Model

2.1. Conservation equations, boundary and initial conditions

The evolution of the composition, temperature and velocity fields for the model problem may be found by solution of the equations expressing conservation of mass, momentum, energy and light component together with an equation of state and an appropriate set of boundary and initial conditions. By adoption of d, κ/d , d^2/κ , $\eta_0 \kappa/d^2$, dq_0/κ and $\Delta C = C_1 - C_0$ as the scales for length, velocity, time, pressure, temperature and composition, respectively, the conservation equations may be written in adimensional form as:

$$\nabla \cdot \boldsymbol{u} = 0 \tag{2}$$

$$\mathbf{0} = -\nabla p + \nabla^2 \mathbf{u} + Rq(T - R\rho C) \mathbf{j}$$
(3)

$$\frac{\mathrm{D}T}{\mathrm{D}t} = \nabla^2 T \tag{4}$$

$$\frac{DC}{Dt} = 0 \tag{5}$$

In writing eqns. (2)-(5), a Boussinesq equation of state of the form

$$\rho = \rho_0 [1 - \alpha (T - T_0) + \beta (C - C_0)]$$
(6)

where ρ_0 is the reference density of fluid at temperature T_0 and composition C_0 has been adopted. The normalized composition appearing in eqn. (5) is the fraction of light component in the two-component fluid. The coefficient β is defined by $\beta = \rho_0^{-1}(\partial \rho / \partial C)$. It is convenient to recall that $\beta \Delta C$ is identical to $\Delta \rho / \rho_0$ where $\Delta \rho$ represents the intrinsic density difference between the fertile (hence dense) material of the transition region and overlying depleted mantle. The fluid is assumed to be incompressible and of infinite Prandtl number ($\Pr = \nu_0 / \kappa$) where ν_0 is

TABLE 1

Notation and values for parameters appropriate for upper mantle mixing

Parameter	Symbol	Units	Value
Acceleration of gravity	 g	(m/s^2)	9.8
Thermal expansion	α	(K^{-1})	2×10^{-5}
Bottom-layer thickness	d_0	(km)	250
Top-layer thickness	d_1	(km)	300
Thermal diffusivity	ĸ	(m^2/s^{-1})	5×10^{-7}
Bottom-layer viscosity	ν_0	(m^2/s^{-1})	2×10^{18}
Thermal conductivity	ĸ	$(J m^{-1} K^{-1} s^{-1})$	3.0
Basal heat flux	q_0	(mW/m^{-2})	33.4

the kinematic viscosity of fluid at $T = T_0$ and $C = C_0$ and is equal to η_0 / ρ_0 .

Inspection of eqns. (2)-(6) reveals that there are two adimensional parameters in this problem. These are the thermal Rayleigh number based on on the imposed heat flux into the transition region:

$$Rq = \frac{g\alpha q_0 d^4}{\kappa k \nu_0} \tag{7}$$

and the ratio of compositional and thermal buoyancy:

$$R_{\rho} = \frac{(\Delta \rho / \rho_0)k}{\alpha q_0 d} = \frac{\beta \Delta C k}{\alpha q_0 d}$$
(8)

All quantities and numerical values are defined in Table 1.

Figure 2 depicts the boundary and initial conditions utilized in the simulations. Note that we ignore the lithospheric lid at d < 100 km in the calculation. The boundary between the lower and upper mantle at a depth of 650 km is a slip surface through which no material enters. A constant basal heat flux, q_0 is imposed there. The computational domain has an aspect ratio of 3:1; reflecting and adiabatic conditions on velocity and temperature, respectively, are assumed to approximate conditions in a low-aspect-ratio layer. The top of the computational domain, which corresponds to the base of the lithosphere, is taken as a rigid, isothermal surface through which no material enters or leaves. At t = 0, the adimensional composition of the upper and lower layers are 1 and 0, respectively; pure light compo-



Fig. 2. Computational domain, boundary and initial conditions for the numerical simulations. Slip conditions for velocity are imposed along the side-walls as well as the base of the computational domain (i.e. along the upper-mantle-lowermantle contact). The top boundary is rigid. Side-walls are adiabatic, the top boundary is isothermal and a constant heat flux (q_0) is imposed on the bottom. All boundaries are impermeable with respect to light component. At t = 0, the fluid is isothermal (T = 0) and motionless. The enriched piclogite layer has thickness 250 km; the depleted harzbugite layer is 300 km thick.

nent is defined by an adimensional composition C = 1. At t = 0, the temperature is set equal to a constant T_0 ; and a constant heat flux q_0 is imposed along y = 0 at the base of the upper mantle at 650 km. Finally, the velocity is set equal to zero at t = 0 everywhere. The choice of initial conditions on T and u are, of course, arbitrary. We are interested mainly in the long-term evolution of the layered arrangement and not transients associated with spin-up from the imposed initial conditions.

2.2. Numerics

The solution to eqns. (2)–(5) subject to the boundary and initial conditions shown in Fig. 2 has been accomplished by means of a Galerkin finite element method as implemented by Sewell (1985). Details of the method may be found in previous works (e.g. Oldenburg et al., 1989; 1990; Rosenberg and Spera, 1990, 1992). Briefly, solutions are obtained using from 1500 to 3000 triangular elements with quadratic basis functions. Advancement of eqns. (3) and (4) is accomplished using a fully implicit time-stepping scheme (Fletcher, 1988). Solution of eqns. (2) and (3) is accomplished by introduction of a penalty parameter such that pressure may be eliminated from the momentum equations. As is well known, when the penalty parameter becomes small, the resulting momentum conservation equations approach the usual Navier-Stokes equations (e.g. Temam, 1968). It is difficult to obtain good solutions to eqn. (4) due to its hyperbolic nature. In order to surmount this problem we have introduced an artificial diffusion term on the right-hand side of eqn. (5) following usual practices. The effect of this procedure is to numerically smear the composition field. Independent numerical experiments were undertaken to evaluate the trade-off between the CPU requirements, the spatial resolution desired for the composition field and the magnitude of the artificial diffusion coefficient. For a typical result presented below, a compositional front moves about 2% of the characteristic length of the domain in several Ga. In the determination of the statistics of compositional mixing, we have averaged over a sufficiently large volume in order to partially overcome this problem. This procedure, while not without shortcomings, has the advantage of enabling solution of the conservation equations without exceedingly excessive CPU requirements.

3. Results

3.1. Field evolutions

In this series of simulations, we seek to establish the style and mechanisms of mixing between the two initially homogeneous layers as a function of $\Delta \rho / \rho_0$. The thermal Rayleigh number, Rq is fixed at 2×10^5 , a value roughly appropriate for the upper mantle (see Table 1) and the fluid is treated as a constant viscosity material.

In Fig. 3, the globally averaged kinetic energy of the flow is plotted against time for values of $\Delta \rho / \rho_0$ equal to 0, 2, 4 and 8%. The adimensional spatially averaged specific kinetic energy defined according to

$$KE = \frac{1}{2} \int_0^3 \int_0^1 (u^2 + v^2) \, \mathrm{d}y \, \mathrm{d}x / \int_0^3 \int_0^1 \, \mathrm{d}y \, \mathrm{d}x$$
(9)



Fig. 3. Temporal evolution of the adimensional spatially averaged kinetic energy (*KE*, defined in eqn. (10)) as a function of intrinsic density difference $\Delta \rho / \rho_0$ between the initially homogeneous layers. It should be noted that the passive mixing case ($\Delta \rho / \rho_0 = 0$) is steady by $t \approx 2.5$ Ga. For $\Delta \rho / \rho_0$ close to the 'critical' value of 0.03, the flow is characterized by largeamplitude oscillations due to reversals in the sense of circulation. The high intrinsic density cases of $\Delta \rho / \rho_0 = 0.04$ and 0.08 exhibit two-layer convection with relatively little mixing of the depleted and enriched reservoirs.

gives a global view of the characteristics and vigor of the flow field. For the passive tracer case $(\Delta \rho / \rho_0 = 0)$, KE approaches a steady value (KE \approx 2000), after transients associated with the initial conditions damp out. The first, large-amplitude peak in the KE time series (Fig. 3) corresponds to be development of vertically extended plumes (Figs. 4(a), 5(a) and 6(a)) that carry hot fluid upwards. The transient oscillation noted on the KE time series has a period of about 0.6 Ga and rapidly damps. By 2-3 Ga, quasi-steady velocity, temperature and passive tracer composition fields are established. The average and maximum temperature within the domain are approximately constant since the convective heat transport balances the imposed basal heat flux for this passive mixing case (see Fig. 5).

Results for non-zero differences in intrinsic density of 2, 4 and 8% show more interesting *KE* time-series behavior (Fig. 3). For $\Delta \rho / \rho_0 = 0.02$, there is a long induction time following an early spike in *KE*. During this interval (1 Ga $\leq t \leq 2$ Ga), enthalpy is stored in the heavy bottom layer

where convection is initially confined due to the effects of intrinsic stratification (see Fig. 4(e)). The obvious effect of increasing the intrinsic density difference is to suppress thermal instabilities from developing along the bottom as they obviously do in the passive mixing case (e.g. compare Fig. 4(a), 4(e) and 5(a) and 5(e)). The planform of convection in this early interval lacks the symmetry observed in the passive scalar case. A comparison of compositional fields between the passive and $\Delta \rho / \rho_0 = 0.02$ cases shows that the interface between the two layers is little deformed during the first Ga of evolution (cf. Figs. 6(a) and 6(e)). At later times ($t \approx 2$ Ga), sufficient thermal buoyancy is present in the bottom layer to overcome the modest (2%) intrinsic density difference. The flow field radically changes for t > 2.5 Ga (Figs. 4(f), 4(g), 5(f), (g), 6(f) and 6(g) and for a period of time, of order 0.5 Ga, a crude form of doublelayer convection occurs (Fig. 4(f)). For t > 3 Ga an aperiodic regime of convection is set up and maintained. In order to investigate more fully the KE and Nusselt number time series, the simulation was carried out much further than shown on Fig. 3. Power spectra of the KE and Nu time series (not shown) exhibit features characteristic of chaotic convection including a broad-band distribution of power, although there is a local maximum in power at a frequency corresponding to a period of roughly 0.5 Ga. The composition field evolved in a manner consistent with expectations; relatively little deformation of the compositional interface during the first 1.5 Ga (Figs. 6(e) and (f) followed by destruction of layering as travelling waves along the compositional interface eventually grow to an amplitude on the order of the layer thickness (e.g. see Figs. 6(g) and (h)). It should also to noted that more heat is stored in the transition zone because of the stabilizing effect of the initial intrinsic density difference. This increases the average and maximum temperature of the upper mantle.

Finally, results are shown in Fig. 3 for the KE time series for $\Delta \rho / \rho_0 = 0.04$ and 0.08. In these cases, the overall evolution of the flow, temperature and composition field are similar although the $\Delta \rho / \rho_0 = 0.04$ case is slightly more vigorous than the $\Delta \rho / \rho_0 = 0.08$ case. Early on $(t \le 1 \text{ Ga})$

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Fig. 4. Temporal evolution of the stream function as a function of time and intrinsic density difference $\Delta \rho / \rho_0$. $\Delta \rho / \rho_0 = 0$ for (a)-(d); $\Delta \rho / \rho_0 = 0.02$ for (e)-(h); $\Delta \rho / \rho_0 = 0.04$ for (i)-(l); and $\Delta \rho / \rho_0 = 0.08$ for (m)-(p). The maximum and minimum stream function value and interval for each frame are as follows: (a) 45, -45, 5; (b) 24, -24, 5; (c) 26, -10, 5; (d) 26, -20, 5; (e) 16, -18, 2; (f) 7, -7, 1; (g) 30, -25, 5; (h) 25, -60, 5; (i) 12, -12, 2; (j) 6, -6, 1; (k) 8, -6, 1; (l) 10, -12, 1; (m) 10, -10, 1; (n) 5, -5, 1; (o) 4, -4, 1; (p) 4, -6, 1. Double-layer convective extends over the age of the Earth provided $\Delta \rho / \rho_0 \equiv 4\%$. The *Rq* number is constant and equal to 2×10^5 .



Fig. 5. Temporal evolution of the temperature field for identical parameters relevant to Fig. 4. $\Delta T = T_{\text{max}} - T_0$ is the maximum temperature difference between the base of the transition zone at 650 km depth and the base of the lithosphere, defined by the isothermal condition $T = T_0$.



Fig. 6. Temporal evolution of the composition field as a function of time and intrinsic density difference for identical parameters relevant to Fig. 4. Isopleths plotted for C = 0.25, 0.5 and 0.75.

convection is confined to the bottom layer since the potential energy associated with the heavy bottom layer dominates. For $t \ge 2$ Ga, however, the enthalpy gradient across the interface is sufficient to initiate weak convection within the upper layer. Examination of Figs. 5(k), 5(l), 4 (k) and 4(1), clearly indicate that circulation within the two layers is shear coupled. Note, for example, from Fig. 5(k), when a bottom-layer plume impinges on the upper layer, a downwelling is induced within the upper layer. This same behavior occurs in the $\Delta \rho / \rho_0 = 0.08$ case, although at a time exceeding the age of the Earth. The evolution of the C-field is quite different in these strongly density-stratified cases compared with the passive and $\Delta \rho / \rho_0 = 0.02$ cases. In particular, there is evidence that the mechanism of mixing is different. As depicted in Fig. 4(1), in the high $\Delta \rho / \rho_0$ regime, the integrity of the interface is never compromised. Mass transfer across the interface occurs by entrainment and not by the penetration of plumes. That is, tendrils of light fluid are sheared and transported by convectively induced viscous stresses similar to the features observed by Olson (1984) in laboratory studies. Compare for instance Figs. 3(b) and 3(c) in Olson to Fig. 4(1) in the present study. Color video animations (available from F.J. Spera) show details that cannot be appreciated in static snapshots. These details are consistent with convectively driven entrainment as noted in laboratory studied for the high $\Delta \rho / \rho_0$ cases.

3.2. Mixing statistics

In order to provide a quantitative basis for assessment of the 'goodness of mixing' between the initially homogeneous layers during convective evolution, we have studied the statistics of mixing utilizing the continuum nature of the mixture. In particular, the variance of the composition field, the first integral of the two-point compositional correlation function as well as the average composition within each of the homogeneous layers has been monitored as a function of time. This approach allows one to recover information regarding the scale and variance of compositional anomalies as a function of $\Delta \rho / \rho_0$ and enables

one to estimate a 'mixing time' based on quantitative criteria. Below we give a rough sketch of the theory, details may be found in Danckwerts (1952) and in Oldenburg et al. (1989).

The 'goodness' or extent of mixing generally refers to two distinct, but related measures. One is the variance of the composition field averaged over the entire mixture at a specific time. Because the light component neither enters nor leaves the computational domain (see Fig. 2), the average concentration of light component in the domain is constant and equal to C_{av} . The variance of the composition field is equal to

$$\sigma^2 = \left(\overline{C - C_{\rm av}}\right)^2 \tag{10}$$

where the overbar signifies that a spatial average over the domain has been taken. Note that σ^2 is directly related to the extent to which molecular diffusion has erased concentration differences in the mixture. Molecular diffusion is not an important process for eradication of mantle heterogeneities of characteristic length greater than O(m) due to low chemical diffusivity values appropriate for the mantle (Kellogg and Turcotte, 1987). However, when sample volumes are significantly larger than the resolution of the compositional field it remains useful to define an adimensional variance, referred to as the intensity (I) to monitor the mixing rate. The intensity of mixing (I) is defined

$$I = \frac{\sigma^2}{C_{\rm av}(1 - C_{\rm av})} \tag{11}$$

It should be noted that the denominator in eqn. (11) is the variance of the compositional field at t = 0, before any mixing has occurred. The intensity of mixing is simply a normalized variance.

A second statistical quantity useful in investigating the extent of mixing is the spatial correlation function, R(r). If C_1 and C_2 are the concentrations of light component at two points separated by a distance r, the two-point normalized correlation function may be defined

$$R(r) = \overline{(C_1 - C_{av})(C_2 - C_{av})} / \sigma^2$$
(12)

where the overbar again implies a spatial average has been taken. It should be noted that the two-point compositional correlation function is identically equal to unity for r equal to zero (perfect two-point correlation) and falls to zero when the relation between the concentration of light components at two locations a distance rapart is random. Because the variance goes to zero as $t \to \infty$ (i.e. the fluid becomes compositionally homogeneous), Oldenburg et al. (1989) found it useful to introduce a modified correlation function $R^*(r) = R(r)\sigma^2$. The modified correlation function tends towards zero in the limit of fluid homogenization since $C = C_{av}$ everywhere.

A length scale based on the integral of the correlation function which is conceptually related to the characteristic size of a chemical heterogeneity may be found by integration of the correlation function over all correlation-pair distances at a given time. The linear scale of segregation is accordingly defined

$$L = \int_{0}^{r=r_{0}} R(r) \, \mathrm{d}r \tag{13}$$

where r_0 is the distance at which a random correlation exists between the composition of fluid at two locations separated by the distance r = r0. By analogy with eqn. (14) one may define a modified linear scale

$$L^* = \int_0^{r=r_0} R^*(r) \, \mathrm{d}r \tag{14}$$

which also refers to the characteristic size of a heterogeneity. Nadav and Tadmor (1973) and Tucker (1981) have shown that for mixing in which diffusion is insignificant, L and L^* contain information regarding the characteristic size of a composition anomaly. The studies of Ottino and Chella (1983) and Danckwerts (1953) discuss theoretical and practical aspects of the mixing and blending of viscous fluids.

3.3. Mixing statistics: applications

In Fig. 7, the intensity (1) and product of the linear segregation scale and variance are plotted against dimensional time for values of the intrinsic density parameter $\Delta \rho / \rho_0$ (0, 2, 4 and 8%) presented in Fig. 4, 5 and 6. In each case, the normalized compositional variance or intensity of segregation (1) is equal to unity at t = 0. For the



Fig. 7. (a) Adimensional variance of the composition field (1) vs. time in Ga. Note the rapidity of compositional homogenization for the passive $(\Delta \rho / \rho_0 = 0)$ case and the slow mixing, mainly by viscous entrainment along the compositional interface for the high intrinsic density cases $(\Delta \rho / \rho_0 = 0.04$ and 0.08). The case $\Delta \rho / \rho_0 = 0.02$ is close to the critical density difference and shows an 'intermediate' evolution. (b) Adimensional scale of heterogeneity as a function of time. Although both high $(\Delta \rho / \rho_0 = 0.04, 0.08)$ and low $(\Delta \rho / \rho_0 = 0)$ intrinsic density cases exhibit monotonic decrease in the scale of heterogeneity, the $\Delta \rho / \rho_0 = 0.02$ case shows a staircase time series. This is associated with the propagation of large-amplitude waves on the compositional interface. The sudden drops in L^* for $t \ge 1.5$ Ga are associated with breaking waves (see text).

high intrinsic density ratio cases $\Delta \rho / \rho_0 = 0.04$ and 0.08, (I) varies linearly with time reflecting the small amount of entrainment of light component due to the action of viscous stresses along and near, the initially interface. It should be noted that dI/dt is somewhat larger for $\Delta \rho / \rho_0$ = 0.04 compared with $\Delta \rho / \rho_0 = 0.08$. This suggests that dI/dt does indeed provide a measure of convectively driven mixing and is not a numerical artifact related to artificial diffusion. The mixing time, defined according to $(dI/dt)^{-1}$ is very long for these cases (of order 20 Ga) and clearly shows that the mass transfer rate between the two layers is geologically insignificant. For the passive mixing case $(\Delta \rho / \rho_0 = 0)$, the evolution of the compositional variance is quite different; exponential rather than linear behavior is indicated after an induction time of order 1 Ga. The e-folding time, a convenient measure of the mixing time is ≈ 1 Ga for passive mixing $(\Delta \rho / \rho_0 = 0)$.

The evolution of the variance for the $\Delta \rho / \rho_0 = 2\%$ case shows aspects of both the high $\Delta \rho / \rho_0$ and passive $(\Delta \rho / \rho_0 = 0)$ mixing cases. For $t \leq 2$ Ga, the variance decreases at a rate virtually identical to that observed for early times in the other cases. However, at about $t \approx 2.5$ Ga, dI/dtincreases abruptly and roughly matches dI/dtfound for the passive mixing case. The abrupt change in slope is physically related to the breakdown of the irregular form of two-layer convection (e.g. see Fig. 4(f)) that characterizes flow in the time interval from roughly 1 to 2 Ga.

Based on these runs, we believe that the variance of the compositional field undergoes an evolution characterized by three epoches. The first is an incubation time during which flow is primarily restricted to the bottom layer with very limited mixing along the compositional interface. The second mixing phase begins when sufficient enthalpy accumulates within the lower, intrinsically dense layer to overcome the stabilizing effects of non-zero $\Delta \rho / \rho_0$. This phase of mixing is characterized by large-amplitude deformation of the interface and for values of $\Delta \rho / \rho_0 \leq 0.02$ involves 'breaking-wave' mixing which enables rapid advectively driven mixing. Finally, at long times asymptotic behavior is noted. This is apparent only in the $\Delta \rho / \rho_0 = 0$ case in Fig. 7(a) and sets in once the size of compositional heterogeneities have been reduced to a diffusive length scale.

In Fig. 7(b), the adimensional scale of heterogeneity L^* is plotted against time. Recall that L^* is related to the length-scale over which compositional correlation exists. Because of the integral relationship between $R^*(r)$ and L^* , at a given time, L^* is a measure of the characteristic size of a compositional anomaly. Initial values are high because the initial C-field is layered. It should be noted that for the cases $\Delta \rho / \rho_0 = 0.08$ and 0.04, there is little reduction in L^* since the integrity of the compositional interface is maintained. In the passive case $(\Delta \rho / \rho_0 = 0)$, however, the rapid destruction of the two-layer system after a short induction period is strikingly apparent. The $\Delta \rho / \rho_0 = 0.02$ cases exhibits interesting behavior that may be physically understood by examination of video animations of the temperature and composition field evolution. The rapid decrease in L^* is associated with the penetration of a plume of chemically heavy fluid into the overlying layer with attendant downward flow of the relatively cold, but intrinsically less dense fluid. Because of the juxtapositioning, L^* decreases during this phase. But since cold fluid exchanges light component far slower than heat, a reversal in the circulation occurs. This is a classic effect associated with double-diffusive convection (e.g. see Oldenburg et al., 1989; Turner, 1991). L^* remains approximately constant (or even increases) during the period of time when cold, light fluid sloshes back to the upper part of the domain. This instability recurs throughout the mixing process a number of times as noted in Fig. 7(b). There is an excellent correlation between peaks on the *KE* time series and the plateaus observed in Fig. 7(b) for the $\Delta \rho / \rho_0 = 0.02$ case.

Finally, in Fig. 8, the average composition within each layer is shown as a function of time. The passive mixing case $(\Delta \rho / \rho_0 = 0)$ is clearly



Fig. 8. Fraction of harzbugite within each layer as a function of time for the four values of $\Delta \rho / \rho_0$ cited earlier. While mixing is rapid in the passive case, the high intrinsic density cases mix only slowly. Mixing behavior near the critical $\Delta \rho / \rho_0$ is non-monotonic. The fraction of fertile mantle in the upper layer varies quasi-periodically with a characteristic period of ca. 0.5 Ga, similar to the supercontinent characteristic lifetime.

characterized by rapid mixing after an incubation period of 0.5 Ga. This period has no geological significance; it is simply a function of the (arbitrary) initial conditions. The steep part of the Cversus t plot does, however, have significance and indicates a mixing time of order 0.5 Ga. For $\Delta \rho / \rho_0 = 2\%$ the mixing time defined by the reciprocal of the slope dC/dt is much longer, of the order of several 2 to 3 Ga. Finally, as shown in Figs. 8(c) and 8(d) for $\Delta \rho / \rho_0 = 4\%$ and 8%, respectively, mixing time exceeds the age of the Earth by a factor of 5 or so. It is obvious from this figure that mixing time is very sensitively dependent upon $\Delta \rho / \rho_0$; a change from $\Delta \rho / \rho_0 =$ 0 to $\Delta \rho / \rho_0 = 3\%$ increases the mixing time from several hundred Ma to the age of the Earth.

Conclusions

Perhaps the most significant result is the determination of a value of $R\rho$ which separates systems that significantly mix on a geologic timescale (within say 2 Ga) and those which remain two-layered over the age of the Earth. The critical value of $R\rho$ is about 1/5. This implies that mixing will be efficient provided

$$\frac{\Delta\rho}{\rho_0} < \left(\frac{\alpha a_0 d}{5k}\right) \tag{15}$$

For typical parameter values (Table 1), applicable to mixing of the upper mantle, $\Delta \rho / \rho_0 < 3\%$ leads to mixing. If one adopts parameters relevant to the entire mantle to address the question of mixing between the lower (d > 670 km) and upper mantle, then the condition for mixing is roughly $\Delta \rho / \rho_0 \le 5 + 2\%$. Lack of precise knowledge of appropriate values for α , k and q_0 precludes a tightly constrained value for $\Delta \rho / \rho_0$ when applying eqn. (15) to the problem of mixing between the upper and lower mantle. However, our results are in accord with those of previous workers who have addressed this problem (Jeanloz and Knittle, 1989; Kellogg, 1991; Olson, 1984).

Secondary conclusions of this study relate to the details of mixing as a function of $R\rho$ (or $\Delta\rho/\rho_0$) at fixed Rq. For values of $\Delta\rho/\rho_0$ slightly less than the critical one, early vigorous convection is confined to the bottom layer. After a short period of time (about 1 to 3% of the thermal diffusion time κ/d^2), a spatially irregular aperiodic form of two-layered convection is set up. During this phase, there is significant mixing between the layers by viscous entrainment. By the end of this phase, travelling waves on the compositional interface have amplitudes of the order of the layer depth. Rapid, essentially catastrophic, mixing occurs when the sloshing waves break (e.g. see Figs. 5(f), (g) (h)); thereafter, chaotic convection prevails due to double-diffusive effects that remain important even to times exceeding the age of the earth. For values of $\Delta \rho / \rho_0$ greater than the critical value, mixing is greatly retarded (see Figs. 8(c) and 8(d)). The period of time in which convection is confined to the lower layer is relatively long (or order 1–1.5 Ga). At later times, convection in the upper layer is set up and appears to be viscously coupled to convection in the lower layer. Upwelling in the lower layer sets up a downwelling immediately above in the top layer (e.g. see Figs. 4(k), 5(k)). For these 'double-layer' cases, the mixing occurs wholly by viscous entrainment, similar to the behavior observed by Kellogg (1991). Plume penetration is highly suppressed by the action of gravity on the relatively large density contrast between the layers.

Note that if the value of $\Delta \rho / \rho_0$ within the upper mantle is close to the critical value determined in this study, then the fraction of fertile component in the depleted (harzburgitic) reservoir within the upper mantle (d < 400 km) in not a monotonically increasing function of time (e.g. Fig. 8(b)). Although, of course there is an overall tendency for fluid in the upper and lower reservoirs to homogenize, the approach towards homogenization occurs in steps with a characteristic period of ≈ 0.5 Ga. Significantly, the characteristic size associated with chemical heterogeneity shows a staircase time series (see Fig. 7(b)) with local periods of minor unmixing. In dinstiction, the variance of the composition field as measured by the intensity is a monotonically decreasing function of time. When discussing 'mixing times' one needs to address both the evolution of the variance as well as the integral of the compositional correlation function to obtain a more detailed picture of the complex process of mixing.

We speculate that because the transition layer is fertile (i.e. contains a significant 'basaltic' fraction), the ca. 0.5 Ga periodicity evident in Fig. 3 (for the close-to-critical case $\Delta \rho / \rho_0 = 0.02$) might be expected to correlate with spikes in the volumetric rate of magma production due to decompression melting and perhaps the disruption and dispersal of supercontinents. Detailed examination of the simulation output in video format clearly shows that periods of high fluid KE correlate with times of enhanced heat transfer and material transport across the compositional interface at the top of the transition zone. Recent geochronological and paleomagnetic studies on several Phanerzoic continental flood basalt provinces show that there have been periods when the local volumetric rate of magma eruption is of order $1-2 \text{ km}^3 \text{ year}^{-1}$. These rates are more than an order of magnitude greater than the volumetric rate of magma eruption of the Hawaiian hot spot averaged over the last 80 Ma. While some have argued that epochs of flood basalt volcanism are due to instabilities of D'' at the core-mantle boundary, it is important to point out that petrologic and geochemical constraints are not sufficiently precise at present to entirely rule out intermittent layer instability at 670 km (Machetel and Weber, 1991) or even shallower depths (e.g. 400 km) as discussed here. It is interesting that the best estimates for the Clapeyron slope of the spinel to perovskite + MgO reaction and for differences in bulk composition between the upper mantle above the transition zone (Anderson, 1989; Jeanloz, 1990), the transition zone and lower mantle lead to values of the buoyancy ratio essentially equal to the critical value for both uppermantle-lower-mantle mixing and for mixing within the upper mantle itself. It must be noted that the unambiguous separation of density effects due to phase transitions from those arising due to differences in bulk composition is, at present, difficult. Additional information on the thermodynamic and transport properties of mantle phases is needed to refine estimates of critical density contrasts due to phase transitions and changes in bulk composition throughout the mantle. Simulations in which the effects of a temperature-composition and pressure-dependent viscosity on the critical buoyancy ratio and the statistics of mixing are currently in progress.

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