The feasibility of thermal and compositional convection in Earth’s inner core

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SUMMARY

Inner core convection, and the corresponding variations in grain size and alignment, has been proposed to explain the complex seismic structure of the inner core, including its anisotropy, lateral variations and the F-layer at the base of the outer core. We develop a parametrized convection model to investigate the possibility of convection in the inner core, focusing on the dominance of the plume mode of convection versus the translation mode. We investigate thermal and compositional convection separately so as to study the end-members of the system. In the thermal case the dominant mode of convection is strongly dependent on the viscosity of the inner core, the magnitude of which is poorly constrained. Furthermore recent estimates of a large core thermal conductivity result in stable thermal stratification, hindering convection. However, an unstable density stratification may arise due to the pressure dependant partition coefficient of certain light elements. We show that this unstable stratification leads to compositionally driven convection, and that inner core translation is likely to be the dominant convective mode due to the low compositional diffusivity. The style of convection resulting from a combination of both thermal and compositional effects is not easy to understand. For reasonable parameter estimates, the stabilizing thermal buoyancy is greater than the destabilizing compositional buoyancy. However we anticipate complex double diffusive processes to occur given the very different thermal and compositional diffusivities.

Key words: Numerical approximations and analysis; Heat flow; Composition of the core.

1 INTRODUCTION

The inner core plays an important role in the dynamics of Earth’s interior and understanding its dynamical state provides new and unique insights into the overall thermal and dynamical evolution of the Earth. As the Earth cools, the inner core grows by solidification of the surrounding fluid outer core (Jacobs 1953), releasing latent heat and light elements that provide a driving force for the geo-dynamo (Lister & Buffett 1995). The thermal and compositional structure of the inner core resulting from its gradual solidification may lead to internal convection (Jeanloz & Wenk 1988; Gubbins et al. 2013). Different modes of convection have been proposed to explain some of the seismically observed features of the inner core (Jeanloz & Wenk 1988; Buffett 2009; Alboussi`ere et al. 2010; Monnereau et al. 2010).

Seismology, being the only method available to directly study the inner core, has revealed the existence of anisotropy (Morelli et al. 1986; Woodhouse et al. 1986) and significant degree 1 lateral variations (Tanaka & Hamaguchi 1997). In particular, the upper inner core is seismically isotropic and has a Western Hemisphere with an approximately 1 per cent slower isotropic P-wave velocity and greater attenuation than in the east (Niu & Wen 2001; Cao & Romanowicz 2004; Waszek et al. 2011). Cylindrical anisotropy—with compressional waves travelling fastest along Earth’s rotation axis and slowest along the equatorial plane—appears from a depth of around 100 km below the inner core boundary (ICB) and is concentrated in a region in the western hemisphere (Tanaka & Hamaguchi 1997; Creager 2000; Garcia & Souriau 2000; Deuss et al. 2010; Irving & Deuss 2011; Lythgoe et al. 2014). The eastern region remains isotropic throughout the inner core (Lythgoe et al. 2014).

The dominant phase of iron at inner core conditions is most likely the hexagonal close packed (hcp) structure (Tateno et al. 2010; Stixrude 2012), which is strongly anisotropic (Stixrude & Cohen 1995; Martorell et al. 2013). It has been suggested that alignment of hcp crystals with Earth’s rotation axis may explain the seismically observed cylindrical anisotropy (Stixrude & Cohen 1995), thus a mechanism is needed to align crystals. The idea that thermal convection in the inner core aligns crystals through dislocation glide was first proposed by Jeanloz & Wenk (1988) and has been extensively studied since. Deguen & Cardin (2011) and Cottaar & Buffett (2012) used numerical thermochemical convection models to investigate the likelihood of high-Rayleigh
number, plume style convection in a growing inner core. Both studies conclude that the inner core is more likely to thermally convect early in its history, but this result is dependent on several poorly constrained parameters, such as the heat flux at the core–mantle boundary (CMB) and the core thermal conductivity. Buffett (2009) investigated the pattern of the flow as convection shuts down and showed that centrifugal acceleration may favour a final convective mode with a degree one pattern aligned with Earth’s rotation axis. However, the simulations of Deguen & Cardin (2011) suggest that there is insufficient stress associated with the last convective mode to produce an observable texture. Deguen et al. (2013) extended the model of Deguen & Cardin (2011) to include the effects of the phase change at the ICB.

Recently, translation of the inner core—a convective mode whereby the whole inner core moves to the east due to enhanced solidification in the Western Hemisphere and melting in the east—was proposed to explain the seismic observations (Alboussière et al. 2010; Monnereau et al. 2010). The seismically observed hemispherical variations in isotropic velocity and attenuation in the upper inner core were explained by the grain growth associated with translation of inner core material (Monnereau et al. 2010; Geballe et al. 2013). Translation may also explain the anomalously low velocity layer at the base of the outer core, known as the F-layer (Souriau & Poupinet 1991; Song & Helmberger 1995; Yu et al. 2005; Zou et al. 2008), as a region of dense melt (Alboussière et al. 2010; Deguen et al. 2014). It is more difficult to explain lateral anisotropic variations since translation causes little or no deformation, but this may be explained by coexisting modes of translation and plume convection (Mizzon & Monnereau 2013).

However, since thermally driven inner core convection was originally proposed, it has been suggested both experimentally and theoretically, that the thermal conductivity of the core is significantly higher than previously thought (Sha & Cohen 2011; de Koker et al. 2012; Pozzo et al. 2012; Gomi et al. 2013; Pozzo et al. 2014). Such high thermal conductivity values imply that thermal convection of the inner core is unlikely. However, the possibility remains that convection could be driven by compositional variations.

Compositional convection requires radial variations in the composition of the inner core. The core mainly consists of iron, but Birch (1952) showed that the outer core also contains a substantial amount of light elements. There is growing support for an outer core containing silicon (Georg et al. 2007; Fitoussi et al. 2009; Ziegler et al. 2010) and oxygen (Badro et al. 2014) with the presence of elements such as sulphur, carbon or hydrogen remaining controversial (Hirose et al. 2013). Although light elements preferentially partition into the outer core (Alfé et al. 2002), a small amount of light elements must remain in the inner core to explain the observed density deficit (Jephcoat & Olson 1987). Gubbins et al. (2013) showed that, due to the temperature dependence of the partition coefficient of certain light elements, the inner core may become unstably stratified during its growth, thereby providing a possible mechanism for inner core convection. Labrosse (2014) also showed that compositional variations in the inner core can lead to unstable stratification, although his exact compositional profiles differ from those of Gubbins et al. (2013).

Previous studies of inner core thermal convection (Buffett 2009; Deguen & Cardin 2011; Cottaar & Buffett 2012; Deguen et al. 2013) used low values of thermal conductivity and assumed that compositional effects were stabilizing. Given the uncertainty in physical properties, it remains unclear whether compositional or thermal convection in the inner core is possible and what the corresponding convective style might be.

In this paper, we develop a parametrized model to investigate the possibility of thermal or compositional convection in the inner core. The model allows us to explore the dominance of the plume mode of convection with cold plumes sinking from the ICB and a passive return flow, versus the translation mode. Thermal and compositional convection are presented separately so as to study the end-members of the system. Section 2 outlines the inner core growth model used, which is based on global heat conservation. The parametrized thermal convection model is presented in Section 3 and the method is adapted for compositional convection in Section 4. We discuss the possible effects due to a combination of both thermal and compositional buoyancy in Section 5.

2 GROWTH OF THE INNER CORE

As the core cools, the intersection of the adiabatic temperature with the liquidus temperature occurs at lower pressures, causing the inner core to grow (Fig. 1). We model the growth of the inner core using the simple core thermal evolution model of Buffett (1996), which is based on global heat conservation. Similar treatments are found in Roberts et al. (2003), Labrosse (2003) and Nimmo (2009). An energy budget for inner core growth equates the heat lost from the core at the CMB to the total energy released in the outer and inner core,

\[ Q_{\text{CMB}} = Q_S + Q_L + Q_G, \]

where \( Q_{\text{CMB}} \) is the total heat flow across the CMB, \( Q_S \) is the heat released by secular cooling of the core, \( Q_L \) represents latent heat released due to solidification of the inner core and \( Q_G \) is the change in gravitational energy associated with the exclusion of light elements at the ICB. Each energy term depends on the rate of inner core growth, \( \dd c/\dd t \), where \( c \) is the radius of the inner core and \( t \) is time, as described in detail in Table 1. We assume for simplicity that \( Q_{\text{CMB}} \) is constant. It has been suggested that radioactive elements, particularly potassium, reside in the core (Murthy & Hall 1970; Roberts et al. 2003), but there is sufficient uncertainty regarding their availability that we neglect any energy contribution from internal heating. We also exclude the effect of a varying core composition on the liquidus, since the uncertainty in the value of CMB heat flux overwhelms this error.

The corresponding growth model for the inner core radius is

\[ \frac{\dd c}{\dd t} = \frac{1}{R} \left[ 2c + \frac{3c^2}{b} \left( G + L \right) \right] = 1 \]

(Buffett et al. 1996), expressed in terms of three parameters, \( R \), \( G \) and \( L \) and the outer core radius, \( b \). The parameter

\[ R = \frac{Q_{\text{CMB}}}{\pi \rho C_p b \Theta_0} \]

is expressed as a function of \( \Theta_0 \),

\[ \Theta_0 = \frac{2\pi G C_p b^2}{3} \left( \frac{\partial T_l}{\partial P} \right) \]

which represents the expected temperature drop on solidifying the entire core, where \( \rho \) is the average inner core density, \( C_p \) is the specific heat capacity, \( G \) is the gravitational constant and \( \partial T_l/\partial P \) and \( \partial T_c/\partial P \) are the liquidus and adiabatic gradients, respectively, which we assume to be constant in the inner core. The dimensionless quantities

\[ \Theta = \frac{2}{5} \frac{G b^2 \Delta \rho}{C_p \Theta_0} \],

\[ \Theta_0 \]
Figure 1. (a) Temperature profile in the present-day inner core. The liquidus \((T_L)\) and adiabatic \((T_a)\) profiles intersect at the inner core boundary (ICB). As the core loses heat, the adiabatic profile decreases \([T_a(t + \delta t)]\) and so the liquidus and adiabat intersect at a lower pressure, hence the inner core grows. (b) Schematic of potential temperature, \(\Theta\), in the inner core for superadiabatic conduction (dashed line) and vigorous plume convection (dotted line), where a thin boundary layer develops below the ICB.

Table 1. Principal energy sources affecting core growth. Parameters are listed in Table 2.

<table>
<thead>
<tr>
<th>Contribution</th>
<th>Expression</th>
</tr>
</thead>
<tbody>
<tr>
<td>Secular cooling</td>
<td>(Q_S \approx \frac{4}{3} \pi b^3 \rho T L \frac{\partial T_L}{\partial P} \frac{\partial T_L}{\partial T} )</td>
</tr>
<tr>
<td>Latent heat</td>
<td>(Q_L \approx 4\pi c^2 \rho L \frac{\partial \rho}{\partial T} )</td>
</tr>
<tr>
<td>Gravitational energy</td>
<td>(Q_G \approx \frac{8}{5} \pi^2 G \rho \Delta \rho b^2 c^2 \frac{\partial \rho}{\partial T} )</td>
</tr>
</tbody>
</table>

\[ L = \frac{L}{C_p \Theta_0}, \quad (6) \]

represent the effects of gravitational energy release due to compositional buoyancy and latent heat release, respectively, where \(\Delta \rho\) is the density jump due to compositional change across the ICB and \(L\) is latent heat. Using parameter values in Table 2, \(L = 0.73\), \(G = 0.22\) and \(R = 6.47 \times 10^{-5} \text{ m}^2 \text{ s}^{-1}\).

Values for \(Q_{\text{CMB}}\) have been estimated from seismic observations of the \(D'\) discontinuity and the Clapeyron slope of the post-perovskite transition (Hernlund et al. 2005) or from the buoyancy flux of thermal plumes (Mittelstaedt & Tackley 2006), leading to a range from 7 to 15 TW. Solving (2) for the inner core radius as a function of time for this range of \(Q_{\text{CMB}}\) estimates, results in a broad range of values for the age of the inner core, between 0.5 and 1.5 Byr (Fig. 2). Recently, Gomi et al. (2013) have advocated for the CMB heat flux to be greater than 10 TW in order to power the dynamo with a high core thermal conductivity, resulting in an inner core that is less than 1 Byr old. This range of parameter estimates not only leads to variability in estimates of the growth history of the inner core, but also to uncertainty in estimates of its dynamic evolution.

Table 2. Inner core parameter values.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Units</th>
<th>Value</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>CMB heat flow</td>
<td>(Q_{\text{CMB}})</td>
<td>W</td>
<td>(11 \times 10^{12})</td>
</tr>
<tr>
<td>ICB temperature</td>
<td>(T_L)</td>
<td>K</td>
<td>5700</td>
</tr>
<tr>
<td>Density</td>
<td>(\rho)</td>
<td>kg m(^{-3})</td>
<td>12 900</td>
</tr>
<tr>
<td>Specific heat</td>
<td>(C_p)</td>
<td>J kg(^{-1}) K(^{-1})</td>
<td>840</td>
</tr>
<tr>
<td>Latent heat</td>
<td>(L)</td>
<td>kJ kg(^{-1})</td>
<td>660</td>
</tr>
<tr>
<td>Thermal expansivity</td>
<td>(\alpha)</td>
<td>K(^{-1})</td>
<td>(1.1 \times 10^{-5})</td>
</tr>
<tr>
<td>Grüneisen parameter</td>
<td>(\gamma)</td>
<td></td>
<td>1.4</td>
</tr>
<tr>
<td>Isothermal bulk modulus</td>
<td>(K_T)</td>
<td>Pa</td>
<td>(1.2 \times 10^{12})</td>
</tr>
<tr>
<td>Liquidus gradient</td>
<td>(\frac{\partial T_L}{\partial P})</td>
<td>K Pa(^{-1})</td>
<td>(1 \times 10^{-8})</td>
</tr>
<tr>
<td>Adiabatic gradient</td>
<td>(\frac{\partial T_a}{\partial P})</td>
<td>K Pa(^{-1})</td>
<td>(6.3 \times 10^{-9})</td>
</tr>
<tr>
<td>Thermal conductivity</td>
<td>(k)</td>
<td>W m(^{-1}) K(^{-1})</td>
<td>(36 - 200)</td>
</tr>
<tr>
<td>Thermal diffusivity</td>
<td>(\kappa)</td>
<td>m(^2) s(^{-1})</td>
<td>(4.2 \times 10^{-6})</td>
</tr>
<tr>
<td>Dynamic viscosity</td>
<td>(\eta)</td>
<td>Pa s</td>
<td>(10^{18})</td>
</tr>
<tr>
<td>Kinematic viscosity</td>
<td>(v)</td>
<td>m(^2) s(^{-1})</td>
<td>(7.8 \times 10^{13})</td>
</tr>
<tr>
<td>Outer core fluid velocity</td>
<td>(u)</td>
<td>m s(^{-1})</td>
<td>(10^{-4})</td>
</tr>
<tr>
<td>Density jump at ICB</td>
<td>(\Delta \rho)</td>
<td>kg m(^{-3})</td>
<td>600</td>
</tr>
<tr>
<td>Present inner core radius</td>
<td>(c_0)</td>
<td>km</td>
<td>1221.5</td>
</tr>
<tr>
<td>Outer core radius</td>
<td>(b)</td>
<td>km</td>
<td>3480</td>
</tr>
<tr>
<td>Gravitational constant</td>
<td>(G)</td>
<td>m(^3) kg(^{-1}) s(^{-2})</td>
<td>(6.674 \times 10^{-11})</td>
</tr>
</tbody>
</table>
3 THERMAL CONVECTION

3.1 Energy balance

For thermal convection to occur in the inner core, its internal temperature gradient must exceed the adiabatic gradient, that is it must be superadiabatic (Fig. 1). During convection the internal temperature then evolves toward an adiabatic gradient. Changes over time in the internal temperature are governed by energy conservation—

\[
\frac{d}{dr} \left( \int_T \rho C_p c^2 \tilde{T}(t) \, dV \right) = \int_T \frac{d}{dt} \rho C_p c^2 \tilde{T}(t) \, dS - \int_T q \, dS, \tag{7}
\]

where \( T \) is the internal core temperature, \( V \) and \( S \) are the volume and surface area of the inner core, respectively, and \( T_c \) is the liquidus temperature at the ICB. We write (7) as

\[
\frac{d}{dr} \int_V \rho C_p c^2 \tilde{T}(t) \, dV = 4\pi c^2 \frac{d}{dt} \rho C_p T_c - 4\pi c^2 \tilde{q}, \tag{8}
\]

where \( \tilde{T} \) and \( \tilde{q} \) are the volume averaged internal temperature and surface averaged radial heat flux, respectively.

\[
\tilde{T}(t) = \frac{1}{4\pi c^3} \int_T T \, dV, \quad \tilde{q} = \frac{1}{4\pi c^2} \int_S q \, dS. \tag{9}
\]

Deviations from the adiabatic thermal profile drive the resulting dynamical response, and so we define a potential temperature,

\[
\Theta(x, t) = T(x, t) - T_c(r, t), \tag{10}
\]

as the difference between the temperature and the adiabatic temperature, \( T_c \), such that the internal temperature is superadiabatic when \( \Theta \) is positive. Note that at the ICB \( \Theta = 0 \). The mean potential temperature,

\[
\bar{\Theta}(t) = \frac{1}{4\pi c^3} \int_T \Theta(x, t) \, dV = \bar{T}(t) - \bar{T}_c(t), \tag{11}
\]

is the volume average of the potential temperature. In order to write the energy balance (8) in terms of the mean potential temperature, we first note that

\[
\frac{d}{dr} \left( \int_0^{c(t)} r^2 T_c(r, t) \, dr \right) = \frac{d}{dr} \left( \int_0^{c(t)} r^2 T_c(r, t) \, dr \right) = \frac{d}{dr} \left( \int_0^{c(t)} r^2 \bar{T}_c \, dr \right) = 4\pi \rho C_p c^2 \bar{T}_c \frac{d}{dt} \int_0^{c(t)} r^2 \bar{T}_c \, dr. \tag{12}
\]

Using (11) and (12), the energy balance (8) is therefore

\[
\frac{d}{dr} \left[ 4\pi \frac{3}{2} \rho C_p c^2 \bar{\Theta}(t) \right] = -4\pi \rho C_p \int_0^{c(t)} r^2 \frac{d}{dr} \bar{T}_c \, dr - 4\pi c^2 \tilde{q}. \tag{13}
\]

Since the adiabat and liquidus intersect at the ICB, \( T_c(c(t), t) = T_l(c(t), t) \), thus

\[
\frac{dT_c}{dt} + \frac{dT_l}{dr} \bigg|_{r=r_c} \frac{dc}{dt} \bigg|_{r=r_c} \frac{d}{dr} \bar{\Theta} = \frac{d}{dr} \bigg|_{r=r_c} \frac{dT_c}{dr} - \frac{dT_l}{dr} \frac{d}{dr} \bar{\Theta} \tag{14}
\]

assuming that \( \frac{dT_l}{dt} = 0 \). We may therefore write the evolution of the adiabatic temperature as

\[
\frac{dT_c}{dt} = \left( \frac{dT_c}{dr} \bigg|_{r=r_c} - \frac{dT_l}{dr} \bigg|_{r=r_c} \right) \frac{d}{dr} \bar{\Theta} \tag{15}
\]

Finally noting that

\[
\frac{dP}{dr} = -\rho g(r) = -\rho g' r, \tag{16}
\]

where \( g' = \frac{d}{dr} \frac{g}{\rho} \), the energy balance may be written as

\[
\frac{d}{dr} \left[ 4\pi \frac{3}{2} \rho C_p c^2 \bar{\Theta}(t) \right] = -4\pi \rho C_p \int_0^{c(t)} r^2 \frac{d}{dr} \bar{T}_c \, dr - 4\pi c^2 \tilde{q}, \tag{17}
\]

assuming that \( \frac{dT_c}{dt} \) and \( \frac{dT_l}{dt} \) are uniform in the inner core. We use (17) to investigate the evolution of the mean potential temperature, \( \Theta \), as the inner core grows. The inner core growth rate, \( \frac{d}{dt} \), is determined from the growth model in Section 2. The mean potential temperature evolves, as the inner core grows, according to the conductive or convective regime determining the radial heat flux, \( \tilde{q} \), as discussed in Section 3.2.

3.2 Modes of heat transfer

The radial heat flux may be primarily conductive, plume convective, or given by the translational mode. Here we examine a simplified, and parametrized, model of the radial heat flux. Our parametrized model is similar to that of Cottaar & Buffett (2012), but includes the effect of inner core translation and we do not assume compositional effects to be stabilizing.

Conduction down the adiabatic gradient provides a significant proportion of the radial heat flux. Therefore we parametrize the total heat flux into two parts: a heat flux due to conduction down the adiabatic gradient \( q_{\text{adiab}} \), and a flux from an additional heat transfer that occurs due to the actual temperature gradient being sub- or superadiabatic \( \tilde{q} \),

\[
\tilde{q} = q_{\text{adiab}} + \tilde{q}. \tag{18}
\]

In order to parametrize the additional heat loss due to the departure of the internal temperature from the adiabatic profile, we first derive asymptotic expressions for the heat flux assuming only one
form of heat transport is occurring, deriving separate expressions for the additional heat transport by conduction ($q_{\text{cond}}$), heat transport by plume convection ($q_{\text{plume}}$), and heat transport by inner core translation ($q_{\text{trans}}$). We then approximate the total heat flux due to a combination of these mechanisms as the direct sum of the three asymptotic expressions,

$$
\tilde{q} = q_{\text{diff}} + q_{\text{plume}} + q_{\text{trans}}.
$$

(19)

The result is a single, simple parametrization of the heat flux that provides a good approximation of the radial heat flux in parameter regimes in which there is a single dominant mode of heat transport. In the transition regions between different modes of heat transport the approximation above will be less accurate (see Appendix A for discussion on the accuracy of this approximation), but we will show that it provides a straightforward method for assessing the dynamical regime to sufficient accuracy, particularly given uncertainties in the material parameters.

In order to rigorously determine the dominant mode of convection, either the stability of each mode with respect to perturbations should be studied, or the full dynamical problem solved numerically. However our approach is to use a simple method, whereby we calculate (19) in order to ascertain the dominant mode of heat transport. This dominant, or largest contributing mode, is interpreted as the mode most likely to be observed in that region of parameter space. For example, we infer that translation is the dominant mode most likely to be observed in that region of parameter space. However our approach is to use a simple method, whereby we should be studied, or the full dynamical problem solved numerically.

3.2.1 Conduction

The heat lost from conduction is given by the sum of the heat lost along the adiabat, $q_{\text{adiabat}}$, and the extra heat lost due to departure of the internal temperature from adiabatic equilibrium, $q_{\text{diff}}$,

$$
q_{\text{cond}} = q_{\text{adiabat}} + q_{\text{diff}},
$$

(20)

and may be evaluated from the temperature gradient at the ICB,

$$
q_{\text{cond}} = -k \left. \frac{\partial T}{\partial r} \right|_{r=c} = -k \left. \frac{\partial P}{\partial r} \right|_{r=c} \frac{\partial T}{\partial P} \bigg|_{\text{ICB}} = k\rho g' c \left. \frac{\partial T}{\partial P} \right|_{\text{ICB}},
$$

(21)

where we assume

$$
P = P_0 - \frac{\rho g' c}{2},
$$

(22)

where $P_0$ is a reference pressure at the centre of the Earth.

For parameters relevant to the inner core the conductive temperature and adiabatic are approximately linear functions of pressure (Buffett 2000), and hence

$$
\Theta = T - T_a = \left( \frac{\partial T}{\partial P} - \frac{\partial T_a}{\partial P} \right) (P - P_{icb}).
$$

(23)

By averaging (23) over the inner core and combining with (22), we find that the internal temperature gradient is given by

$$
\frac{\partial T}{\partial P} = \frac{\partial T_a}{\partial P} + \frac{5\Theta}{\rho g' c^2}.
$$

(24)

Thus the conductive heat flux, $q_{\text{cond}}$, may be expressed in terms of the adiabat and the potential temperature

$$
q_{\text{cond}} = k\rho g' c \frac{\partial T}{\partial P} = k\rho g' c \frac{\partial T_a}{\partial P} + 5k \Theta c^{-2}.
$$

(25)

where we define the heat lost by diffusion along the adiabat as

$$
q_{\text{adiabat}} = k\rho g' c \frac{\partial T_a}{\partial P},
$$

(26)

and the heat lost by diffusion due to the departure of the internal temperature from the adiabat as

$$
q_{\text{diff}} = 5k \Theta c^{-2}.
$$

(27)

3.2.2 Plume convection

We next derive an expression for the heat flux from vigorous, plume convection, $q_{\text{plume}}$ [see Deguen & Cardin (2011) and Cottaar & Buffett (2012)]. The convective flux, $q_{\text{plume}}$, is parametrized following conventional scaling arguments that relate the Nusselt number,

$$
\text{Nu} = \frac{q_{\text{plume}}}{q_{\text{diff}}},
$$

(28)

which is a non-dimensional measure of the convective flux, to the Rayleigh number,

$$
\text{Ra} = \frac{\alpha g(c)\Theta_1 c^3}{\kappa v}.
$$

(29)

Here $\alpha$ is the coefficient of thermal expansion, $g(c)$ is the gravitational acceleration at the ICB, $\kappa$ is the thermal diffusivity and $v$ is the kinematic viscosity. For $\text{Ra} \gg \text{Ra}_c$ we use the conventional scaling relationship $\text{Nu} \sim \text{Ra}^{1/3}$, where $\text{Ra}_c$ is the critical Rayleigh number, above which convection occurs. This scaling relationship is based on the assumption that the timescale for convective overturn is small compared to any other timescales in the problem. In this high Ra regime the convective plume flux may be approximated as

$$
q_{\text{plume}} = B k \left( \frac{g' \alpha}{\kappa v} \right)^{1/3} c^{1/3} \Theta_1^{2/3},
$$

(30)

where $q_{\text{plume}} = 0$ when $\Theta < 0$ and $B = 0.48$ is a constant that is taken from the scaling laws derived from the numerical calculations of Deguen et al. (2013). This is similar to the value of $B = 0.49$ found from the numerical simulations of Cottaar & Buffett (2012).

3.2.3 Translation

Finally we derive the average radial heat flux due to inner core translation, $q_{\text{trans}}$. Translation, where the whole inner core moves at a uniform velocity, was first described by Alboissière et al. (2010) and Monnereau et al. (2010). The inner core is displaced
from its equilibrium position such that the ICB temperature does not correspond to the solidus and becomes unstable, resulting in melting on one side and crystallization on the opposite side of the inner core. Topography is removed by phase change and restored by isostatic adjustment towards gravitational equilibrium.

We express the heat lost from translation using the analytical model of Alboussiére et al. (2010), derived from a global force balance on the inner core. Thermal translation requires that the inner core has a global superadiabatic profile that is linear in the translation direction

\[ \frac{\partial \Theta}{\partial x} = A, \]

where \( x \) is aligned with the axis of translation and \( A \) is a constant. At the ICB \( \Theta = 0 \) (ignoring a thin boundary layer on the melting side), so for \( x < 0 \)

\[ \Theta = A \left( r \cos \theta + \sqrt{c^2 - r^2 \sin^2 \theta} \right), \]

where \( \theta \) is the angle between the \( x \)-axis and the point on the ICB. The mean potential temperature may now be written as

\[ \bar{\Theta} = \frac{3A}{4\pi c} \int_{r=0}^{\infty} \int_{\theta=0}^{\pi} \left( r \cos \theta + \sqrt{c^2 - r^2 \sin^2 \theta} \right) \times r^2 \sin \theta \, dr \, d\theta \, d\phi = \frac{3Ac}{4}, \]

hence,

\[ \frac{\partial \Theta}{\partial x} = \frac{4\bar{\Theta}}{3c} \]

The translation velocity governs the rate of crystallization or melting and so the heat flux due to translation,

\[ q_{\text{trans}} = \rho C_p \Theta V i, \]

is proportional to the translational velocity, \( V \), where \( q_{\text{trans}} \) is the heat flux and \( i \) is a unit vector in the translation direction. The total heat loss from translation over the surface, \( S \), of the inner core is therefore

\[ Q_{\text{trans}} = \int_{S} q_{\text{trans}} \cdot n \, dS = \int_{S} \nabla \cdot q_{\text{trans}} \, dV, \]

where \( n \) is the unit normal to the surface. Combining (34–36), the total heat loss over the surface of the inner core is therefore

\[ Q_{\text{trans}} = \rho C_p V \int \frac{\partial \Theta}{\partial x} \, dV = \frac{16\pi}{9} \rho C_p V c^2 \bar{\Theta}, \]

and the corresponding average radial heat flux is

\[ q_{\text{trans}} = \frac{4}{9} \rho C_p V \bar{\Theta}. \]

We follow the derivation of Alboussiére et al. (2010) to find an expression for the translation velocity. The displacement, \( \delta \), of the inner core from an equilibrium position of uniform density can be expressed as a function of the thermal gradient, \( \partial \Theta / \partial x \),

\[ \delta = \frac{\alpha \rho c^2}{5\Delta \rho} \frac{\partial \Theta}{\partial x}, \]

This displacement causes a temperature difference, \( \delta T \), between the liquidus and the adiabat along the ICB

\[ \delta T = \rho_l g(c) \delta \cos \theta \left( \frac{\partial T_L}{\partial P} - \frac{\partial T_a}{\partial P} \right), \]

where \( \rho_l \) is the density of the outer core. The temperature change, \( \delta T \), creates a thermal boundary layer in the outer core, with heat transfer proportional to \( \alpha C_p \delta T \), where \( u \approx 10^{-4} \text{ m s}^{-1} \) (Bloxham & Jackson 1991) is the outer core fluid velocity near the ICB (assumed to be the same order of magnitude as the fluid velocity at the CMB). The heat transfer is accommodated by latent heat associated with the phase change along the boundary

\[ L V \cos \theta = u C_p \delta T. \]

Combining (39)–(41), the translation velocity is given by

\[ V = \frac{4\pi G u C_p \rho_l^2}{15L\Delta \rho} \alpha c^3 \frac{\partial \Theta}{\partial x} \left( \frac{\partial T_L}{\partial P} - \frac{\partial T_a}{\partial P} \right), \]

Using (4) and (34), we rewrite the velocity as

\[ V = \frac{8}{15} \frac{u C_p \rho_l \alpha \Theta_0}{\Delta \rho} \left( \frac{c}{\bar{\rho}} \right)^2, \]

and substituting (43) into (38), the average radial heat flux due to translation is written

\[ q_{\text{trans}} = \frac{32}{135} \frac{u C_p \rho_l \alpha \Theta_0}{\Delta \rho} \left( \frac{c}{\bar{\rho}} \right)^2 \bar{\Theta}^2, \]

where \( q_{\text{trans}} = 0 \) when \( \bar{\Theta} = 0 \). This expression for the translation velocity is strictly only valid in the limit of a rigid inner core since it does not account for isostatic adjustment made via a secondary flow that acts to redistribute degree 1 density anomalies if the viscosity of the inner core is sufficiently low (Deguen et al. 2013). The effect of this on the transition from translation to plume convection is discussed in Appendix A.

### 3.3 Summary of governing equations

We have developed expressions for all contributions to the radial heat flux from the ICB and now summarize the governing equations. We re-arrange the global energy balance of (17)

\[ \frac{d}{dt} \left[ \frac{4\pi}{3} \rho C_p c^3 \bar{\Theta}(t) \right] = \frac{4\pi}{3} \rho C_p c^3 S - 4\pi c^2 \ddot{q}, \]

such that conduction down the adiabat, \( q_{\text{adiabas}} \), is written as part of the source function, \( S \),

\[ S = \rho g c \frac{d}{dt} \left( \frac{\partial T_L}{\partial P} - \frac{\partial T_a}{\partial P} \right) - 3\kappa g \rho c \frac{\partial T_a}{\partial P}, \]

as defined by Deguen et al. (2013). The radial flux, \( \ddot{q} \), defined in (19), only contains terms that depend on the mean potential temperature, \( \bar{\Theta} \), with the diffusive, plume and translational fluxes given by (27), (30) and (44), respectively, with the limit \( \bar{\Theta} = 0 \) when \( \bar{\Theta} = 0 \). We solve the global energy balance of (45) for \( \bar{\Theta} \) by making it dimensionless and combining with the growth model of (2) (Appendix B).

#### 3.3.1 Quasi-steady state approximation

Lastly, by assuming that convection within the inner core is vigorous we can derive expressions that allow comparison of our results to previous work. With this assumption, the time scale of thermal relaxation due to convection (i.e. the time taken for a convective system to return to thermal equilibrium after any changes to the heat flux) is fast compared to the time scale of inner core growth, so the system is in a quasi-steady state. In this limit the dominant energy balance in (45) is between terms \( \frac{4\pi}{3} \rho C_p c^3 S \) and \( 4\pi c^2 \ddot{q} \), thus

\[ \ddot{q} \sim \frac{\rho C_p c S}{3}. \]
If plume convection is dominant, we use $q_{\text{plume}}$ in (47) to write $\Theta$ analytically

$$\Theta \sim \left( \frac{1}{3B} \right)^\frac{1}{4} \left( \frac{v \nu S^3}{k_g \alpha} \right)^\frac{1}{4}.$$  

(48)

This expression is compared to the scaling laws derived from the numerical models of Deguen et al. (2013) [Table 3, Deguen et al. (2013)] in order to determine the value of $B$ that is used in (30). Alternatively if translation is dominant we can compare our results to that of Alboussi`ere et al. (2010). Assuming translation is dominant we use $q_{\text{trans}}$ in (47) to write

$$\Theta \sim \left( \frac{135}{96} \left( \frac{b^2 L \Delta \rho}{c C_p u\rho \alpha \theta_1} \right)^\frac{1}{2} \right).$$

(49)

Substituting this approximate expression for $\Theta$ in the translation velocity (43), we get

$$\nu^2 \sim \frac{4\pi}{15} \frac{G\mu C\rho^2 \nu}{L \Delta \rho} \left( \frac{\partial T_a}{\partial P} - \frac{\partial T_b}{\partial P} \right) S \ell^3$$

(50)

which matches the expression for translation velocity given by Alboussi`ere et al. (2010).

### 3.3.2 Comparison to full solution of governing equations

We use the quasi-steady state approximation above to find expressions for when each mode of heat transport is dominant in order to plot a regime diagram at a particular instance in time. Our regime diagram is compared to the regime diagram calculated by solving the full system of governing equations from Deguen et al. (2013), to allow us to understand the accuracy of our simple, parametrized model. In order to compare our models, we first non-dimensionalize each heat flux term, as detailed in Appendix C. Fig. 3 shows our regime diagram, alongside that from Deguen et al. (2013), plotted for the Rayleigh number defined by Deguen et al. (2013), $\text{Ra}_d$, as

$$\text{Ra}_d = \frac{ag\ell c^6 S}{6k_g \nu},$$

(51)

versus the dimensionless ‘phase change’ parameter, $\mathcal{P}$, defined by Deguen et al. (2013) as

$$\mathcal{P} = \frac{L \Delta \rho g b^2 c}{2 \rho G u \ell \alpha C_P}.$$  

(52)

The dimensionless parameter $\mathcal{P}$ is the ratio of topographic production through solidification melting to viscous relaxation of induced topography. Hence $\mathcal{P}$ governs the type of convection that is dominant, with translation being dominant for low values of $\mathcal{P}$, while plume convection is dominant for high values of $\mathcal{P}$ and $\text{Ra}_d$ (Fig. 3).

We define one mode of heat transfer to be dominant when its flux has the largest contribution to the total heat flux (Table 3), defined by Deguen et al. (2013) as $\text{Ra}_d \sim 103$, while Deguen et al. (2013) obtain $1.5 \times 10^3$, and our estimate of the transition from diffusion to translation is $\text{Ra}_d \approx 211 \mathcal{P}$, while Deguen et al. (2013) obtain $\text{Ra}_d \approx 88 \mathcal{P}$.

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**Figure 3.** Regime diagrams plotted for the Rayleigh number, $\text{Ra}_d$, versus the parameter, $\mathcal{P}$, defined by Deguen et al. (2013). (a) Regime diagram for this study calculated using the quasi-steady state approximation detailed in Appendix C. Dashed lines show when one mode of heat flux is equal to the sum of the other two modes—that is the dashed yellow line indicates when the flux from translation is equal to the sum of the plume and diffusive fluxes. Solid lines indicate when one mode is greater than the other two (Table 3). (b) Regime diagram from Deguen et al. (2013) calculated for the full set of governing equations [see fig. 13a, Deguen et al. (2013)].
Interestingly, we also find a weak dependence of the transition from the plume mode to the translation mode on the Rayleigh number, with a scaling of $\text{Ra}_d \simeq 7.87P^2$ in the asymptotic limit. It is unclear if this dependence was also found in the study of Deguen et al. (2013) since they found a broad region where translation was important (up to $P \sim 1000$). Additionally their study used Rayleigh numbers less than $10^7$ only, therefore to confirm this dependence their analysis would need to be extended to higher values of $\text{Ra}_d$. The different scalings may be due to different definitions of the transition from translation to plume dominant convection, between our parameterized model and the numerical model of Deguen et al. (2013). Deguen et al. (2013) define the transition from translation to plume modes to be the point at which small scale convective flow first emerges, which they interpret as being due to negative feedback of secondary flow on the translation mode. However, our definition is based on heat flux, and the transition from translation to plume modes occurs when the heat flux from plume convection is the largest contribution to the total flux, with the heat flux following the scaling in (30). This transition is discussed more fully in Appendix A.

### 3.4 Thermal results

We now use the theory derived above to study the different modes of thermal convection in the inner core. For comparison with previous studies, Fig. 4 shows the thermal evolution of the inner core for a low thermal conductivity value of $36 \text{ W m}^{-1} \text{ K}^{-1}$ (Stacey & Davis 2008), calculated by solving the energy balance (45) for the mean potential temperature, $\bar{\Theta}$. For a $Q_{\text{CMB}} = 11$ TW and a viscosity of $\mu = 10^{18} \text{ Pa s}$, $\bar{\Theta}$ is positive at all times, increasing as the size of the inner core grows, then decreasing as the rate of inner core growth slows (Fig. 4a). A lower value of CMB heat flux (e.g. $Q_{\text{CMB}} = 7$ TW, dotted line, Fig. 4a) allows more time for heat to dissipate from the inner core, causing $\bar{\Theta} \to 0$ and any convection to stop at an earlier stage of inner core evolution, in agreement with Deguen & Cardin (2011) and Cottaar & Buffett (2012).

To investigate the dominant mode of convection, the average radial heat flux from the inner core is calculated for each convective mode, using eqs (27), (30) and (44). The average radial heat flux follows a similar pattern to the mean potential temperature, first rising then decreasing. Translation is the dominant mode, except when the inner core is very young when diffusion dominates (Fig. 4b). The corresponding translation velocity is on the order of $10^{-10} \text{ m s}^{-1}$ (Fig. 4c), around three times greater than the inner core growth rate, which is the minimum velocity at which seismic observations can be explained by translation (Monnereau et al. 2010). We also show the translation velocity calculated in the quasi-steady state approximation (dashed line, Fig. 4c), which was used in the study by Alboussi`ere et al. (2010). The quasi-steady state approximation causes an overestimation of the translation velocity compared to our model which does not require this approximation. We therefore use our solution in the remaining calculations.

We have used a representative CMB heat flux value of 11 TW, which fits within recent constraints (Lay et al. 2008; Gomi et al. 2013). Thermal convection does not occur for a $Q_{\text{CMB}}$ less than approximately 6 TW, assuming a thermal conductivity of $36 \text{ W m}^{-1} \text{ K}^{-1}$. For thermal convection to occur for higher thermal conductivity values, greater values of $Q_{\text{CMB}}$ are required. For example a thermal conductivity of 200 W m$^{-1}$ K$^{-1}$ requires $Q_{\text{CMB}} \gtrsim 32$ TW for the inner core to be thermally unstable ($\bar{\Theta} > 0$) and convect.

An important parameter is the viscosity of the inner core which is poorly determined with published values ranging from $10^{11}$ Pa s (Van Orman 2004) to $10^{22}$ Pa s (Reaman et al. 2011). Thermal conductivity estimates have also changed significantly, from around $36 \text{ W m}^{-1} \text{ K}^{-1}$ (Stacey & Davis 2008) to over $200 \text{ W m}^{-1} \text{ K}^{-1}$ (de Kokker et al. 2012; Pozzo et al. 2012). Therefore Fig. 5(a) shows the dominant convective style for a range of inner core viscosity and thermal conductivity values, estimated by comparing the radial heat flux for each convective mode. The strength of plume convection ($q_{\text{plume}}$) versus translation ($q_{\text{trans}}$) is strongly dependent on the viscosity of the inner core (Figs 5b–d), with translation being dominant for viscosities above approximately $10^{18} \text{ Pa s}$, in agreement with Alboussi`ere et al. (2010) and Deguen et al. (2013). Greater thermal conductivities cause convection to shut off at smaller inner core radii since the inner core becomes subadiabatic (Fig. 5e), until

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**Figure 4.** Thermal evolution of the inner core for parameter values in Table 2, with $k = 36 \text{ W m}^{-1} \text{ K}^{-1}$ and $Q_{\text{CMB}} = 11$ TW. (a) Mean potential temperature, $\bar{\Theta}$, calculated numerically (solid line), with $Q_{\text{CMB}} = 7$ TW (dotted line) for comparison, and using the quasi-steady state approximation (with $Q_{\text{CMB}} = 11$ TW, dashed line). (b) Heat flux lost by diffusion (cyan), plume convection (magenta) and translation (yellow). (c) Translation velocity calculated numerically (solid line) and using the quasi-steady state approximation (dashed line).
Figure 5. (a) Dominant convective mode for a range of estimated inner core viscosity and thermal conductivity values (using $Q_{CMB} = 11$ TW), with colours corresponding to the amount of time the inner core has spent in each mode. Profiles for several thermal conductivity and viscosity values are shown for: (b) $k = 40 \text{ W m}^{-1} \text{ K}^{-1}, \eta = 10^{14} \text{ Pa s}$; (c) $k = 40 \text{ W m}^{-1} \text{ K}^{-1}, \eta = 10^{18} \text{ Pa s}$; (d) $k = 40 \text{ W m}^{-1} \text{ K}^{-1}, \eta = 10^{21} \text{ Pa s}$; (e) $k = 60 \text{ W m}^{-1} \text{ K}^{-1}, \eta = 10^{18} \text{ Pa s}$.

Thermal convection cannot occur for thermal conductivities greater than $68 \text{ W m}^{-1} \text{ K}^{-1}$ (Fig. 5a). Given that the most recent estimates for core thermal conductivity are between approximately 150 and 240 W m$^{-1}$ K$^{-1}$ (Sha & Cohen 2011; de Koker et al. 2012; Pozzo et al. 2012, 2014; Gomi et al. 2013), thermal convection will not have occurred at any point in the inner core’s lifetime. However, as we will show in Section 4, compositional stratification may provide an alternative driving force for inner core convection.

4 COMPOSITIONAL CONVECTION

The seismically observed density jump at the ICB is too large to be explained solely by the density difference between the solid and liquid phase transition of iron and therefore requires enrichment of light elements in the fluid outer core relative to the solid inner core (Alfè et al. 2002). Jephcoat & Olson (1987) first showed that the inner core must also contain light elements due to the density deficit of the inner core with respect to the density of pure iron, with the main candidate light elements thought to be oxygen, sulphur and silicon (Hirose et al. 2013). Alfè et al. (2002) use ab initio calculations to examine the partitioning of sulphur, oxygen and silicon between solid and liquid at core conditions, estimating the light element concentration needed to match the seismically constrained ICB density jump. Their calculations show that oxygen partitions strongly from solid to liquid, while slightly more sulphur partitions into the liquid than the solid and silicon partitions equally between both phases.

In view of the fact that thermal convection in the inner core is unlikely for large estimates of the thermal conductivity, it is important to investigate the possibility of compositionally driven convection.
It has previously been assumed that compositional variations in the inner core are stably stratified, hindering convection (Deguen & Cardin 2011; Cottaar & Buffett 2012). The stable stratification is the result of a constant partition coefficient over time, such that more light elements solidify in the inner core as the outer core concentration increases over time. However, Gubbins et al. (2013) recently showed that the light element concentration in the inner core may actually decrease as the inner core grows, because the partition coefficient is temperature dependent. In the case of sulphur and oxygen, this may result in a decreasing light element concentration with inner core radius, causing unstable stratification (Gubbins et al. 2013). Since silicon partitions equally between solid and liquid, its concentration does not change with time.

We first define the chemical potential, $\mu$, of a phase in a multi-component system following Alfé et al. (2002),

$$\mu = \mu^0 + \lambda \chi + k_B T \ln \chi,$$  

where $\mu^0$ and $\lambda$ are constants obtained from ab initio calculations, and represent a reference chemical potential and a linear correction from ab initio calculations, respectively (Alfé et al. 2002), $k_B$ is Boltzmann’s constant, and $\chi$ is the molar ratio. Equilibrium at the solidification interface requires that the solid and liquid chemical potentials are equal, $\mu_s = \mu_l$, thus

$$\mu_s^0 + \lambda_s \chi_s(c) + k_B T_s \ln \chi_s(c) = \mu_l^0 + \lambda_l \chi_l(c) + k_B T_l \ln \chi_l(c),$$

where $\chi$ is the molar ratio at the solidification interface, denoted by superscript $i$ and subscripts $s$ and $l$ represent solid and liquid, respectively. The partition coefficient, $P_{ul}$, is the ratio of solid and liquid mole ratios at the ICB,

$$P_{ul} = \frac{\chi_s(c)}{\chi_l(c)} = \exp \left[ \frac{\mu_s^0 + \lambda_s \chi_s(c) - \mu_l^0 - \lambda_l \chi_l(c)}{k_B T(c)} \right],$$

which is non-linear in $\chi_s$ and $\chi_l$. The smaller the partition coefficient, the less light elements crystallize into the inner core. Due to the dependence of the partition coefficient on the liquidus, $T_l$, which is in turn dependent on pressure, the composition of material added to the inner core changes as the inner core grows. As in (23) we assume that the temperature gradient with pressure is constant and so express the liquidus at the ICB, $T_l(c)$, as a function of core radius by

$$T_l(c) = T_l(c_0) + \frac{1}{2} \frac{\partial T_l}{\partial P} \rho_s(c_0^2 - c^2),$$

where $c_0$ is the present-day inner core radius. We neglect the effect of composition on the liquidus, since Labrosse (2014) showed this to be small.

We solve for the solid composition at the ICB, $\chi_s(c)$, by first assuming that the outer core is well mixed, such that the mean liquid composition, $\bar{\chi}_l$, equals the liquid composition at the solidification interface

$$\bar{\chi}_l(c) = \chi_s(c).$$

and so write the solid composition at the ICB explicitly in terms of the mean liquid concentration by re-arranging (55),

$$\chi_s(c) = \frac{k_B T_l(c)}{\lambda_s} \left[ \bar{\chi}_l(c) \lambda_s - \bar{\chi}_l(c) \lambda_s \right] \exp \left[ \frac{\lambda_s \bar{\chi}_l(c) + \mu_s^0 - \mu_l^0}{k_B T_l(c)} \right],$$

where $\bar{\chi}_l$ is calculated from present day inner and outer core concentrations obtained from seismology (Table 4).

The validity of our assumption of a well-mixed outer core is somewhat uncertain, although if the seismically observed F-layer is a global, density-stratified layer, the analysis will hold assuming partitioning occurs over a layer of fluid (Gubbins et al. 2013).

4.1 Mass balance

We now construct a mass balance for light elements using an analogous approach to that used for heat in Section 3.1. Equating the change in total moles of light element in the inner core with moles added at the ICB minus moles lost by diffusion and convection we obtain

$$\frac{d}{dt} \left[ 4\pi \frac{3}{2} \rho_c \bar{\rho} \bar{c}_l \right] = 4\pi \rho_s c^2 \frac{d}{dt} \chi_s(t) \frac{M}{M} - 4\pi \rho c^2 q_m,$$

where $q_m$ is the molar flux and $M$ is the average molar mass of the inner core.

Likewise, we now define a potential composition,

$$\phi(x, t) = \chi_s(x, t) - \chi_s',$$

as the difference between the light element composition in the inner core, $\chi_s$, and the composition added at the ICB, $\chi_s'$, in a manner analogous to the potential temperature, such that $\phi > 0$ for convection to occur. The mean potential composition is defined as the volume average

$$\bar{\phi}(t) = \frac{1}{2\pi c^3} \int \phi(r, t) dV = \bar{\chi}_l(t) - \chi_s'(t).$$
Writing the mass conservation (60) in terms of the mean potential composition,

$$\frac{d}{dt} \left( \frac{4\pi}{3} \frac{\rho}{M} \ell \phi \right) = \frac{4\pi}{3} \frac{\rho}{M} S_\ell - 4\pi c^2 q_m,$$  

we obtain an equation which is analogous to the thermal energy balance in (45), using the source function from Deguen et al. (2013),

$$S_\ell = -\frac{d\chi_i^\ell}{dt},$$  

which represents the change in composition of material added to the inner core as it grows.

Since the source term, (64), depends on the concentration in the outer core, we solve for the composition at the ICB, $\chi_i^\ell$, and the potential composition, $\phi$, simultaneously. This is done by making the mass conservation eq. (63) dimensionless, and applying the non-dimensional growth model (Appendix D1). The dimensionless eq. (D1) is then solved together with (58), (59) and (62) as a system of differential algebraic equations (Appendix D2). A comparable treatment is performed by Labrosse (2014). Gubbins et al. (2013) simplify the problem by assuming that changes in the internal composition, $\chi_i^\ell$, are small, allowing variations in the liquid concentration, $\bar{\chi}_l$, hence variations in the concentration added to the inner core, $\chi_i^\ell$, to be calculated analytically (using (59) and (58), respectively). Before solving for $\chi_i^\ell$ and $\phi$ we derive expressions for the radial molar flux, $q_m$, from the inner core as detailed below.

### 4.2 Modes of molar flux

We again approximate the radial flux to be the sum of contributions from compositional diffusion ($q_{\text{diff}}$), plume convection ($q_{\text{plume}}$) and translation ($q_{\text{trans}}$),

$$q_m = q_{\text{diff}} + q_{\text{plume}} + q_{\text{trans}},$$

where $q_m$ corresponds to molar flux. We find expressions for each molar flux term independently as a function of mean potential compositional, in a directly analogous manner to the thermal case discussed in Section 3.2.

#### 4.2.1 Diffusion

The diffusive radial flux is now parametrized using Fick’s law for compositional diffusion, so that the compositional diffusive flux is

$$q_{\text{diff}} = -D \left. \frac{\partial \Phi}{\partial r} \right|_{r_{\text{ICB}}} = \frac{5D \Phi}{c},$$

in analogy to (27), where $D$ is the solid diffusivity and $\Phi$ is the average potential molar concentration

$$\Phi = \frac{\bar{\phi} \rho}{M}.$$  

#### 4.2.2 Plume convection

For the plume mode of convection a compositional Rayleigh number,

$$R_{\text{comp}} = \frac{\alpha_c g(c) \bar{\phi}(c) c^3}{D\nu},$$

may be defined, where $\alpha_c$ is the compositional expansion coefficient. We assume the same high Ra scaling, $R_{\text{comp}} \sim R_{\text{comp}}^2$, and so express the convective flux from plume convection as

$$q_{\text{plume}} = \frac{BD \rho}{M} \left( \frac{g' \alpha_c}{\nu D} \right)^{1/3} c^{1/3} \phi^{4/3},$$

where we use $B = 0.48$ as before.

#### 4.2.3 Translation

The analysis for the translation model based on potential temperature can be adapted for compositional effects (Deguen et al. 2013). In this instance density variations in the inner core arise from differences in the composition of the melting and crystallizing sides of the inner core, causing a displacement in its centre of mass. Following the analysis for potential temperature in Section 3.2.3, the molar flux from translation is

$$q_{\text{trans}} = \frac{4}{9} \frac{\rho}{M} V \bar{\phi}.$$  

The rate of translation remains limited by the ability of the outer core to remove heat at the ICB and so the translation velocity is expressed

$$V = \frac{8}{15} \frac{uC_p \rho c \Theta_0}{L \Delta \rho} \bar{\phi} \left( \frac{\bar{\phi}^3}{\bar{b}^3} \right).$$

### 4.3 Compositional results

We now use the theory above to study the different modes of compositional convection. We show results for sulphur and oxygen separately due to the uncertainty in core composition and since they may be considered as end members of a more complex Fe–O–S–Si system. We use present day core concentrations calculated for the ICB density jump obtained from the radially symmetric PREM model (Dziewonski & Anderson 1981). Calculations have also been performed for the model of Masters & Gubbins (2003), however we show only PREM values since we are interested in compositional variations over time and the PREM density jump is consistent with other Earth models (Kennett & Engdahl 1991; Kennett et al. 1995).

Figs 6 and 7 show the evolution and convective influence of sulphur and oxygen in the core, respectively. The concentration of sulphur in the outer core increases as the inner core grows since the partition coefficient is less than 1 (Fig. 6a). However the increase in liquid concentration trades off with the decrease in the partition coefficient as the ICB moves to lower pressures, causing the concentration of sulphur added at the ICB to decrease initially. The sulphur concentration begins to increase when the inner core has a radius of around 550 km (Fig. 6b). The initial decrease of $\chi_i^\ell$ creates a positive potential composition (Fig. 6c), which then decreases until it becomes negative at a radius of around 650 km. If there is no inner core convection ($q_{\text{plume}} = q_{\text{trans}} = 0$) the potential composition is slightly greater and becomes negative at a later time (dashed line, Fig. 6c). Fig. 6(d) shows that while the potential composition is positive, the inner core is convecting, with translation being the dominant mode with a translation velocity on the order of $10^{-11}$ m s$^{-1}$ (Fig. 6e).

The oxygen concentration also increases in the outer core as the inner core grows (Fig. 7a). However unlike sulphur, the oxygen concentration added at the ICB continuously decreases (Fig. 7b), resulting in a positive potential composition and an inner core that is still convecting today (Figs 7c and d). The dominant convective mode is translation, with a translation velocity on the order of $10^{-10}$ m s$^{-1}$ (Fig. 7c), which is similar to the rate of thermally driven translation.
Figure 6. Evolution of sulphur with increasing radius of the inner core with parameter values from Tables 2 and 4. (a) Outer core composition, $\bar{\chi}_l$. (b) Solid composition at the ICB, $\chi_s^l$, from (58) (solid line) and using the approximations of Gubbins et al. (2013) (dashed line). (c) Potential composition in the inner core, $\bar{\phi}$, with (solid line) and without (dashed line) inner core convection. (d) Flux from diffusion (cyan), plume convection (magenta) and translation (yellow). (e) Translation velocity.

Figure 7. Evolution of oxygen with increasing radius of the inner core with parameter values from Tables 2 and 4. (a) Outer core composition, $\bar{\chi}_l$. (b) Solid composition at the ICB, $\chi_s^l$, from (58) (solid line) and using the approximations of Gubbins et al. (2013) (dashed line). (c) Potential composition in the inner core, $\bar{\phi}$, with (solid line) and without (dashed line) inner core convection. (d) Flux from diffusion (cyan), plume convection (magenta) and translation (yellow). (e) Translation velocity.
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Figure 8. (a) Dominant convective mode for a range of estimated inner core viscosity and sulphur solid diffusivity values, with colours corresponding to the amount of time the inner core has spent in each mode. Profiles for several diffusivity and viscosity values are shown for (b) \( D_s = 10^{-9} \text{ m}^2 \text{ s}^{-1}, \eta = 10^{11} \text{ Pa s} \) and (c) \( D_s = 5 \times 10^{-13} \text{ m}^2 \text{ s}^{-1}, \eta = 10^{20} \text{ Pa s} \).

Figure 9. (a) Dominant convective mode for a range of estimated inner core viscosity and oxygen solid diffusivity values, with colours corresponding to the amount of time the inner core has spent in each mode. Profiles for several diffusivity and viscosity values are shown for (b) \( D_o = 10^{-9} \text{ m}^2 \text{ s}^{-1}, \eta = 10^{11} \text{ Pa s} \) and (c) \( D_o = 5 \times 10^{-13} \text{ m}^2 \text{ s}^{-1}, \eta = 10^{20} \text{ Pa s} \).

Gubbins et al. (2013) and Labrosse (2014) also solved for the inner core interface composition, but their studies found differing solutions for a seemingly unresolved reason (Labrosse 2014). We match the results of Labrosse (2014), however find we can also match the results of Gubbins et al. (2013) by changing the treatment of the chemical potential at the solidification interface (dotted line, Figs 6ba and 7b). Gubbins et al. (2013) assume present day compositions when calculating the partition coefficient (see eq. 55), while Labrosse (2014) update the interface composition as the system evolves, which is the correct treatment. In the case of oxygen, Gubbins et al. (2013) also neglected the linear \textit{ab initio} corrections.

The solid diffusivity of sulphur and oxygen at core conditions is uncertain, with values likely to be less than that of the liquid [around \( 10^{-9} \text{ m}^2 \text{ s}^{-1} \) Gubbins et al. (2013)]. Figs 8 and 9 show the model space for a range of mass diffusivity and inner core viscosity values, for sulphur and oxygen, respectively. It is clear that translation is the dominant mode, except if the inner core viscosity is low and the diffusivity is high when plume convection dominates while the inner core is young.

5 COMBINED THERMAL AND COMPOSITIONAL EFFECTS

The convection resulting from solely thermal or compositional effects is now well understood, with our analysis showing that translation is likely to be the dominant convective style, particularly for compositional convection. However it is not trivial to understand the style of convection arising from a combination of both thermal and compositional diffusion.

Labrosse (2014) argues that the total buoyancy can be approximated from the sum of all thermal and compositional effects,

\[
\delta \rho/\rho_{\text{ICB}} = \alpha_s \dot{\theta} + \alpha_o \dot{\phi}_o + \alpha_s \dot{\phi}_s, \tag{72}
\]

where superscripts \( s \) and \( o \) correspond to sulphur and oxygen, respectively and \( \delta \rho/\rho_{\text{ICB}} > 0 \). We calculate this density anomaly for several thermal conductivity values and a combination of thermal and compositional effects using results from our end-member simulations, as shown in Fig. 10. The density anomaly is primarily controlled by the thermal instability and is always negative for a thermal conductivity of 75 W m\(^{-1}\) K\(^{-1}\) or greater, independent of the inclusion of compositional effects.

However, we note that even if the net density gradient is stabilizing, convection may occur through double diffusive convection [convection driven by two components with different rates of diffusion, see Huppert & Turner (1981)] since the rates of thermal and compositional diffusion differ by approximately \( 10^6 \). For instance, if the thermal conductivity is very large, any temperature anomalies will rapidly dissipate leading to a uniform thermal field, leaving only the possibility of compositionally driven convection remaining. Therefore it is possible that compositional convection may play the dominant role, particularly given the uncertainty in thermal conductivity estimates for the inner core.
approximately greater than $10^{18} \text{ Pa s}$ (Fig. 5).

Recent estimates. In the case of thermal convection, translation is likely to occur for higher thermal conductivity values requires the CMB heat flux to be greater than 30 TW, which is significantly higher than recent estimates. In the case of thermal convection, translation is the dominant mode for an inner core with a high viscosity, approximately greater than $10^{13} \text{ Pa s}$ (Fig. 5).

A wide range of values for the viscosity of the inner core have been estimated, ranging from $10^{17}$ to $10^{22} \text{ Pa s}$ (Dumberry & Bloxham 2002; Van Orman 2004; Reaman et al. 2011). The most recent estimates of $10^{17} \text{ Pa s}$ and $10^{13}...10^{18} \text{ Pa s}$ come from length of day variations (Davies et al. 2014) and from mineral physics experiments (Gleason & Mao 2013), respectively. The uncertainty in the viscosity of the inner core causes uncertainty in the type of convection occurring in the inner core, particularly for thermal convection.

We have also shown that compositional stratification can provide another driving force for convection in the inner core. Oxygen always generates an unstable density profile (Fig. 6), while sulphur generates an unstable profile until the inner core reaches a radius of approximately 650 km, when it becomes stabilizing (Fig. 7). For both oxygen and sulphur, translation is the likely mode of convection, although there is a weak dependence on viscosity and diffusivity (Figs 8 and 9).

The value of the solid diffusivity of sulphur and oxygen at core conditions is uncertain, although it is likely to be less than the liquid diffusivity. This low diffusivity favours translation of the inner core and so uncertainty in the inner core viscosity is less important for compositional convection (Figs 8 and 9) than for thermal convection.

The translation velocity, for translation driven by variations in temperature and oxygen composition, is sufficient to explain the seismic structure of the upper inner core according to the model of Monnereau et al. (2010). However, since the rate of translation is primarily controlled by the ability of the outer core to extract or provide heat at the ICB, a change in the outer core fluid velocity also changes the translation velocity by the same amount. Thus if the outer core fluid velocity at the ICB is one order of magnitude less than that at the CMB (the estimate that is currently used), then the rate of translation will be too slow to explain the lateral variations in the upper inner core.

The composition of the core is still controversial and we consider only the model of Alfè et al. (2002), based on the average earth model of PREM (Dziewonski & Anderson 1981) in this work, since all relevant parameters are given. This choice was sufficient for our study since our primary aim was to demonstrate that compositional variations in the inner core over time may drive inner core convection. However better knowledge of the composition of the core is needed before definitive conclusions regarding inner core convection can be drawn.

There is also large uncertainty in the remaining core parameters, significantly in the CMB heat flux, which controls the rate at which the core cools and the inner core grows. In order to narrow the parameter space, better constraints on these important parameters are needed.

Lastly, even if translation is occurring in the inner core, an explanation for lateral anisotropy variations still remains elusive. The most likely explanation for cylindrical anisotropy is the bulk alignment of intrinsically anisotropic crystals, thus a mechanism is needed to generate crystal alignment in the western ‘hemisphere’, with random bulk crystal alignment in the remaining inner core. Since very little deformation accompanies translation of the inner core, it is unlikely that translation will generate crystal alignment. It is possible that translation could be accompanied by another mechanism that orients crystals, such as preferred equatorial solidification (Yoshida et al. 1996), or deformation due to Maxwell stresses (Karato 1999; Buffett & Wenk 2001). However any accompanying deformation mechanisms would need to work in an inner core with a high viscosity, since this is required for inner core translation.

### 6 DISCUSSION

We have shown that thermal convection occurs in the inner core for a thermal conductivity less than approximately $68 \text{ W m}^{-1} \text{ K}^{-1}$ (assuming parameters from Table 2). However this value depends on the assumed value of CMB heat flux and is also sensitive to uncertainties in outer core properties, significantly the difference between the Clapeyron and adiabatic gradients. For thermal convection to occur for higher thermal conductivity values requires the CMB heat flux to be greater than $10^{17} \text{ Pa s}$ and $10^{15}...10^{18} \text{ Pa s}$ come from length of day variations (Davies et al. 2014) and from mineral physics experiments (Gleason & Mao 2013), respectively. The uncertainty in the viscosity of the inner core causes uncertainty in the type of convection occurring in the inner core, particularly for thermal convection.

We have also shown that compositional stratification can provide another driving force for convection in the inner core. Oxygen always generates an unstable density profile (Fig. 6), while sulphur generates an unstable profile until the inner core reaches a radius of approximately 650 km, when it becomes stabilizing (Fig. 7). For both oxygen and sulphur, translation is the likely mode of convection, although there is a weak dependence on viscosity and diffusivity (Figs 8 and 9).

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### 7 CONCLUSIONS

The parameterized convection model we present approximates the total heat or compositional flux from the inner core as the sum of the heat or composition lost through conduction, plume convection and translation. We use our parameterized model to study the likelihood of either thermal or compositional convection in the inner core and assume the dominant convective mode to be the greatest contribution to the total flux. We find that thermal convection is unlikely to occur for the most recent estimates of core thermal conductivity unless the CMB heat flux is unreasonably large. However a translating convective mode may be driven in the inner core by compositional variations. By simply linearly combining the thermal and compositional buoyancy it appears that the inner core is stably stratified, unless the thermal conductivity is small. We suggest that future work might profitably focus on the possible double diffusive effects, that are often complex and unexpected (Huppert &
Turner 1981), arising from a combination of both thermal and compositional buoyancy, potentially still making inner core convection feasible.

ACKNOWLEDGEMENTS

We would like to thank Chris Davies for help with comparison to his results, plus Deputy Editor Stéphane Labrosse, Renaud Deguen and an anonymous reviewer for constructive comments that improved the manuscript. KHL and AD are funded by the European Research Council under the European Community’s Seventh Framework Programme (FP7/2007-2013)/ERC grant agreement number 204995. JAN is partially funded by a Royal Society University Research Fellowship.

REFERENCES


**APPENDIX A: VALIDITY OF THE HEAT FLUX PARAMETRIZATION**

In this work, we have chosen to parametrize the heat flux as a direct sum of terms representing heat flux due to conduction, plume convection and translation. Each of these terms are given by asymptotic expressions which formally only apply when a single mode of heat transport dominates. Consequently, our direct sum heat flux parametrization will accurately estimate the heat flux in the parameter regimes where a single mode of heat transport dominates, but may be a poor approximation in the transition regions between modes.

Fig. A1 shows an example of the potential benefits and shortcomings of our approach. The observed Nusselt number–Rayleigh number relationship for a series of 2-D numerical simulations of plume convection by McKenzie et al. (1974) is plotted in red. In these simulations the Nusselt number, Nu, is 1 until the critical Rayleigh number (Ra) is reached (the onset of convection), at which point the Nusselt number steadily increases with increasing Rayleigh number as convection becomes more vigorous. At large Rayleigh numbers there is an asymptotic scaling of Nu ∼ B Raα with B = 0.23. The Nusselt number–Rayleigh number relationship given by our direct sum parametrization of the heat flux is plotted in blue, which yields Nu = 1 + B Raα. In this case our approximation overestimates the heat flux by up to a factor of 3, with the approximation being poorest near the critical Rayleigh number and best at the extremes of large and small Rayleigh number.

We use the direct sum approximation to determine the dominant mode of heat transport, by assuming that the form of heat transport with the largest contribution to the total heat flux is that which is dominant. In the context of Fig. A1, this means that any regime with Nu > 2 is considered plume-convolution-dominated, and anything with Nu < 2 is diffusion-dominated. This transition happens at a particular critical Rayleigh number Ra_c ∼ 100 shown in blue, slightly less than the true critical Rayleigh number for convection Ra_c ∼ 657 shown in red. It is important to note that the
transition between conduction and convection is controlled by the correct dimensionless parameter (the Rayleigh number), and only the numerical value of the transition point differs. Thus our direct sum parametrization is likely to be a good guide to the true behaviour of the system, at the very least in an order-of-magnitude sense.

We also investigate the accuracy of our direct sum parametrization by looking at the transition from translation to plume dominated convection. The numerical simulations of Deguen et al. (2013) show that this transition is governed by the emergence of secondary flow and smaller scale convection. The secondary flow redistributes the hemispherical density anomalies associated with translation, decreasing the strength of translation until the translation mode disappears.

Fig. A2 shows the variation of normalized translation velocity versus the phase change parameter, \( \mathcal{P} \), from (52). We define the normalized translation velocity, \( V/\Theta_0 \),

\[
\frac{V}{\Theta_0} = \frac{8}{\sqrt{30}} \sqrt{\frac{R_a}{\mathcal{P}}} \Theta',
\]

where \( V \) is the translation rate from (43) and \( \Theta_0 \) is the quasi-steady state translation rate from (50). We calculate (A1) using \( \Theta' \) obtained assuming the vigorous convection approximation in (C9) for given values of \( R_a \) and \( \mathcal{P} \) (Fig. A2 is plotted for \( R_a/\mathcal{P} = 10^5 \)). As Fig. A2(a) shows, the rate of translation slows as \( \mathcal{P} \) increases, since the plume mode of convection emerges (blue dots). Also plotted is the \( O(\mathcal{P}) \) analytical solution of Deguen et al. (2013) (black line), which again shows a decrease in the translation rate with increasing \( \mathcal{P} \), but with a much sharper drop off. This is because our parametrized model does not account for secondary flow which is an intermediate regime occurring in the transition between translation and plume convection and this results in an overestimate of the strength of translation at large \( \mathcal{P} \).

Fig. A2(b) shows the average radial heat flux due to translation, divided by the total radial heat flux due to translation and plume convection. This decreases as \( \mathcal{P} \) increases, since translation becomes less vigorous. We define the transition from translation to plume dominated convection to be when the heat flux from translation is greater than a combination of other modes, that is when \( \eta_{\text{trans}}/(\eta_{\text{trans}} + \eta_{\text{plume}}) = 0.5 \). This transition occurs when \( \mathcal{P} \approx 10^4 \) for \( R_a/\mathcal{P} = 10^5 \) (blue dashed line, Fig. A2b), although the critical value of \( \mathcal{P} \) changes with \( R_a/\mathcal{P} \). In contrast Deguen et al. (2013) find the transition from translation to plume modes to be independent of \( R_a \) and so occurs at approximately \( \mathcal{P} \approx 29 \). Deguen et al.’s (2013) value is when the mean degree of kinetic energy becomes greater than 1, that is when smaller scale convective modes first appear. This definition of the transition from translation to plume modes is different from ours, which is based on heat flux. We define the transition to be the point at which plume convection is dominant and obeys the asymptotic scaling relationship \( Nu \sim Ra^{2/3} \); Deguen et al. (2013) define the transition term is of the shape of internal flow and is when the first small-scale modes emerge.

A more accurate parametrization of the heat flux that more closely resembles the heat flux relationships seen in numerical solutions to the full set of governing equations (such as those by Deguen et al. 2013) would be favourable. However, constructing such a parametrization is non-trivial and is a topic for future work. Nevertheless, we expect that the simple direct sum parametrization we use here has captured the leading-order-behaviour of the system, which is most important given the large uncertainties in parameter values.

APPENDIX B: NON-DIMENSIONAL GROWTH AND THERMAL MODEL

We solve our model as a system of non-dimensional equations as outlined below, using the thermal scalings given in Table B1. We non-dimensionalize (2) to express the inner core growth model as

\[
\frac{1}{\eta} \frac{d\eta'}{d\eta} = \mathcal{M}[2 + 3\eta(G + \mathcal{L})].
\]
where $\Theta'$ is the dimensionless 'phase change' parameter from Deguen et al. (2013), defined in (52). From (C4), we know that
\[ \tilde{q} = \tilde{q}_{\text{diff}} + \tilde{q}_{\text{plume}} + \tilde{q}_{\text{trans}} = \frac{1}{3}. \] (C9)

The boundaries between the three regimes are defined as
\[ \tilde{q}_{\text{diff}} = \tilde{q}_{\text{plume}}, \] (C10)
\[ \tilde{q}_{\text{diff}} = \tilde{q}_{\text{trans}}, \] (C11)
and
\[ \tilde{q}_{\text{plume}} = \tilde{q}_{\text{trans}}. \] (C12)

In order to highlight the transition areas between regimes, we also calculated the boundaries when one mode is equal to the sum of the remaining two modes, that is
\[ \tilde{q}_{\text{diff}} = \tilde{q}_{\text{plume}} + \tilde{q}_{\text{trans}} = \frac{1}{6}, \] (C13)
\[ \tilde{q}_{\text{plume}} = \tilde{q}_{\text{diff}} + \tilde{q}_{\text{trans}} = \frac{1}{6}, \] (C14)
and
\[ \tilde{q}_{\text{trans}} = \tilde{q}_{\text{diff}} + \tilde{q}_{\text{plume}} = \frac{1}{6}. \] (C15)

We solve for the regime boundaries numerically to plot the regime diagram, of $\text{Ra}$ versus $\mathcal{P}$ in Fig. 3. To calculate the regime boundaries (solid lines, Fig. 3a) we solve for (C9) together with one of (C10), (C11) or (C12) depending on the boundary of interest. To calculate the boundaries when one mode becomes dominant (when the mode is equal to the sum of the remaining modes, dashed lines, Fig. 3a), we first solve for $\Theta'$ using a given value of $\text{Ra}$ and either one of (C6), (C7) or (C8) depending on the regime we are interested in.

The critical value of $\mathcal{P}$ is then calculated from one of (C13), (C14) or (C15).

### APPENDIX D: NON-DIMENSIONAL COMPOSITIONAL MODEL

**D1 Compositional convection**

As for the thermal model, we non-dimensionalize the governing equation, (63), this time using the compositional scalings in

\[ \tilde{q} = \frac{q}{\rho C_p c S} = \frac{\rho C_p c S}{3 \rho C_p c S} = \frac{1}{3}, \] (C4)
Table B1 and we combine with the growth model in (B1), such that the governing equation becomes

\[ \frac{d\bar{\phi}}{d\eta} = -S_c - \frac{3\bar{\phi}}{\eta} - 3q'_m \mathcal{M}_c [2 + 3\eta(\bar{G} + \mathcal{L})]. \]  

(D1)

\( q'_m \) is the molar flux due to diffusion, plume convection and translation

\[ q'_m = q'_{\text{diff}} + q'_{\text{plume}} + q'_{\text{trans}} \]  

(D2)

where

\[ q'_{\text{diff}} = \frac{5\bar{\phi}}{\eta} \]  

(D3)

\[ q'_{\text{plume}} = B \mathcal{R}_a \frac{1}{4} \bar{\phi}^2 \eta \]  

(D4)

\[ q'_{\text{trans}} = \frac{32}{135} H_c \eta^2 \bar{\phi}^2 \]  

(D5)

and

\[ \mathcal{R}_a = \frac{g' b_A c}{v D}, \quad H_c = \frac{a C_p q_a b \Theta_0}{L \Delta \rho D}. \]  

(D6)

The non-dimensional translation velocity is

\[ \nu' = \frac{8}{15} H_c \eta^2 \bar{\phi}. \]  

(D7)

D2 Solution to compositional convection

We solve the governing compositional convection equations as a system of differential algebraic equations. First, we substitute (62)—re-arranged for the average inner core composition, \( \bar{\chi}_s \)—into (59) such that the mean liquid composition, \( \bar{\chi}_l \), is a function of the mean potential composition, \( \bar{\phi} \), that is

\[ \bar{\chi}_l = \chi_0 - \frac{\eta}{3} \bar{\chi}_s + \frac{\eta}{3} \left( \bar{\chi}_0 - \eta (\bar{\phi} + \chi'_{i}) \right). \]  

(D8)

This expression for \( \bar{\chi}_l \) is now substituted into (58) in order to remove the dependence of \( \chi'_{i} \) on \( \bar{\chi}_l \)

\[ \chi'_{i}(c) = \left( \frac{k_B T_L(c)}{\lambda_i} \right) \times \mathcal{W} \left[ \chi_0 - \frac{\eta}{3} (\bar{\phi} + \chi'_{i}) \lambda_i \left( \sum \frac{k_B T_L(c)(1 - \eta^3)}{k_B T_L(c)(1 - \eta)} \right) \exp \left( \frac{\lambda_i k_B T_L(c)}{k_B T_L(c)(1 - \eta^3)} \right) \right]. \]  

(D9)

Finally, we re-write the governing eq. (D1) as

\[ \frac{d\bar{\phi}}{d\eta} + \frac{d\chi'_{i}}{d\eta} = -\frac{3\bar{\phi}}{\eta} - 3q'_m \mathcal{M}_c [2 + 3\eta(\bar{G} + \mathcal{L})] \]  

(D10)

in order to solve for \( \bar{\phi} \) and \( \chi'_{i} \) by casting (D9) and (D10) as a system of differential algebraic equations.