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Can the Earth's dynamo run on heat alone?

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SUMMARY

The power required to drive the geodynamo places significant constraints on the heat passing across the core–mantle boundary and the Earth's thermal history. Calculations to date have been limited by inaccuracies in the properties of liquid iron mixtures at core pressures and temperatures. Here we re-examine the problem of core energetics in the light of new first-principles calculations for the properties of liquid iron.

There is disagreement on the fate of gravitational energy released by contraction on cooling. We show that only a small fraction of this energy, that associated with heating resulting from changes in pressure, is available to drive convection and the dynamo. This leaves two very simple equations in the cooling rate and radioactive heating, one yielding the heat flux out of the core and the other the entropy gain of electrical and thermal dissipation, the two main dissipative processes.

This paper is restricted to thermal convection in a pure iron core; compositional convection in a liquid iron mixture is considered in a companion paper. We show that heat sources alone are unlikely to be adequate to power the geodynamo because they require a rapid secular cooling rate, which implies a very young inner core, or a combination of cooling and substantial radioactive heating, which requires a very large heat flux across the core–mantle boundary. A simple calculation with no inner core shows even higher heat fluxes are required in the absence of latent heat before the inner core formed.

Key words: core convection, first-principles calculations, geodynamo, thermal history.

1 INTRODUCTION

The existence of a geomagnetic field places a constraint on the Earth's thermal history. Any model of the Earth's evolution must involve sufficient heat loss from the core to power the dynamo, but not so much as to freeze the core too quickly. These dual constraints are surprisingly strong.

Electrical resistance produces a continual drain of energy that must come ultimately from the Earth's internal heat, gravitational energy, radioactive heating and, depending on the dynamo mechanism, rotational energy. Early studies invoked radioactive heating as the source of thermal convection in the core, and recognized that heat would be converted into magnetic energy with a Carnot-type thermodynamic efficiency (Bullard 1950). Verhoogen (1961) invoked latent heat of freezing of iron in the core as the main source of heat. Braginsky (1963) proposed compositional convection driven by separation of a light component of the outer core mix by freezing.

Backus (1975) and Hewitt *et al.* (1975) showed that the thermodynamic 'efficiency' could be estimated from the entropy balance in the core and, surprisingly, could exceed unity because the electrical heating remains within the core: it is not useful work exported by the heat engine. Gubbins (1977) used the entropy method to show that gravitational energy released by compositional convection was converted to magnetic energy with far greater thermodynamic efficiency than heat, with the details depending on the chemical potential. Loper (1978) computed the energies released by a cooling, differentiating core, and Gubbins *et al.* (1979) used entropy balance to establish dynamo maintenance with reasonable cooling rates and core parameters.

Gubbins (1977) and Gubbins *et al.* (1979) showed that gravitational energy released by contraction in a hydrostatic, adiabatic state is taken up almost entirely by work done in compression, and is therefore not available to drive the dynamo. Häge & Müller (1979) performed a rather sophisticated calculation of the shrinkage accompanying cooling, and concluded that gravitational energy released by freezing of iron is a significant additional power source for the geodynamo not considered by previous studies (see also Müller & Häge 1979). We reiterate here that gravitational energy changes due

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to thermal contraction and, equivalently, volume change on freezing, do not enter the entropy balance and are therefore not available to drive the dynamo. Furthermore, we show here that the pressure heating associated with volume change on freezing is equal to the additional latent heat released by the effect of the pressure change on the melting temperature and consequently the inner core radius.

Mollett (1984) computed a more complete thermal history for the Earth using parametrized convection to account for mantle cooling and found that, for several choices of parameters, the inner core reached its present radius relatively early and then evolved much more slowly. More recent calculations by Buffett *et al.* (1996), Labrosse *et al.* (1997) and Stacey & Stacey (1999) all suggest the inner core is a rather recent feature, forming at about 2 Ga.

Ultimately, all of these calculations rely on estimates of the properties of the material that makes up the inner and outer cores. Seismology provides excellent estimates of the seismic velocities, compressibilities and density. The remaining quantities have so far come from high-pressure experiments on iron and extrapolations of known properties to high pressures and temperatures (Anderson & Ahrens 1994). Data are scarce for solid iron and almost non-existent for liquid iron and iron alloyed with lighter elements such as oxygen, silicon and sulphur, candidate materials for the light component in the outer core.

Theoretical calculations are now able to predict the properties of iron (Alfè *et al.* 1999a, 2000a; Vočadlo *et al.* 1999) and liquid iron mixtures (Alfè & Gillan 1998; Alfè *et al.* 1999b, 2000b, 2002a, 2002b) at core pressures and temperatures. The results add credence to estimates of some of the common properties of iron used in earlier calculations. We therefore revisit the thermal history calculations to see what difference the new parameter estimates make. The work is reported in two stages: this paper describes results for a one-component core with a dynamo driven purely by thermal convection. In a companion paper we give results for binary mixtures in which compositional convection contributes to the geodynamo. This paper gives us the opportunity to review the theory without the complications of two chemically reacting components, and to investigate claims that additional gravitational energy sources allow thermal convection to drive the geodynamo alone.

2 GROSS THERMODYNAMICS OF THE CORE

The model is developed more rigorously in this and the next section. Some of this is a repetition of Gubbins *et al.* (1979); this is necessary to clarify some obscure parts of that paper, correct some minor errors and extend the discussion of gravitational energy released by volume change on freezing. Lister & Buffett (1995) and Buffett *et al.* (1996) have challenged the original treatment of gravitational energy lost by contraction but this now seems to be based on a misunderstanding of the original papers; Lister (2003) has now shown their method gives the same global equations as are used here.

2.1 The basic state

We are interested in the slow evolution of the Earth in general, and of the core in particular. For many purposes the core can be approximated by a stationary fluid in hydrostatic equilibrium with an adiabatic temperature. This state slowly evolves with time as the Earth cools and contracts. Contraction implies a very slow, downward radial motion of the material, denoted by $\mathbf{u}$. Superimposed on this basic state is the convection. Averaging over some intermediate time that is long compared with the lifetime of a convective cell but short compared with the Earth's slow evolution, is assumed to produce the basic state: the pressure p averages to hydrostatic, the temperature T averages to adiabatic, the gravitational potential ψ, defined by $\mathbf{g} = +\nabla\phi$, where $\mathbf{g}$ is acceleration due to gravity, averages to that for a spherically symmetric density distribution, etc. The entire core fluid flow, convective plus contractive, is denoted by $\mathbf{v}$, to distinguish it from the slow contraction, $\mathbf{u}$. We do not distinguish between convective and basic state values of the other variables; no confusion should arise from this. The reader is referred to Braginsky & Roberts (1995) for the most complete discussion of this basic state.

In previous work the fluid flow was assumed to average to $\mathbf{u}$, but this is an unnecessary restriction. For example, a steady convective flow driven or influenced by boundary temperature anomalies may persist on the long timescale used here. Such a flow does not affect the gravitational or internal energy provided departures from adiabatic temperature and hydrostatic pressure are small. Slow changes in the convective pattern change the kinetic energy but the contribution to the total power budget is negligible. Henceforth we shall assume that $\mathbf{v}$ averages to $\mathbf{u}$, the slow contraction, and ignore any long-term convective pattern.

It is possible to estimate gross thermodynamic properties of the core in terms of the basic state. The convection still determines the results through its influence on the quasi-steady basic state: maintaining a well-mixed adiabatic core; generating a magnetic field, etc.; but we do not need to know the details. Products of the convective quantities do not average to give basic state values. An important example is $\mathbf{v}\cdot\nabla p$, the rate of working by the fluid against pressure forces. It is tempting but wrong to replace this with $\rho\mathbf{u}\cdot\nabla\psi$ using the equation for hydrostatic pressure

$$\nabla p = \rho\nabla\psi, \tag{1}$$

where ρ is the density and ψ is the gravitational potential.

Estimation of the integrals that describe the gross thermodynamics is therefore rather subtle. They are manipulated using the equation of mass conservation

$$\frac{\partial\rho}{\partial t} + \nabla\cdot(\rho\mathbf{v}) = 0 \tag{2}$$

and Reynolds' transport theorem for an integral over a material volume

$$\frac{d}{dt}\int \rho A\, dV = \int \rho\frac{DA}{Dt}dV \tag{3}$$

$$= \int \rho\left(\frac{\partial A}{\partial t} + \mathbf{v}\cdot\nabla A\right)dV \tag{4}$$

$$= \int \frac{\partial(\rho A)}{\partial t}dV + \oint \rho A\mathbf{v}\cdot d\mathbf{S} \tag{5}$$

Reynolds' transport theorem relates the total rate of change of a property of an entire volume of material (A) to the volumetric rates of change of that quantity at points inside it. Form (5) clearly separates the contribution of changes within the volume from that of flow across the boundary.

The time average of an integral such as $d/dt\int\rho A\, dV$ can be estimated using the basic state because it is the rate of change of a gross property of the entire material volume. Form (4) suggests that it depends on a product of $\mathbf{v}$ and gradients of A, but the contribution of this fluctuating part to the long-term evolution, must average to zero. Form (5) confirms this: the boundary is a material surface and therefore $\mathbf{v}\cdot d\mathbf{S} = \mathbf{u}\cdot d\mathbf{S}$.

2.2 The energy equation

The equation for energy conservation at a point is

$$\frac{\partial}{\partial t}\left(\rho e+\frac{1}{2}\rho\mathbf{v}^2+\frac{\mathbf{B}^2}{2\mu_0}\right)=-\nabla\cdot\left[\rho\mathbf{v}\left(\frac{1}{2}\mathbf{v}^2+e+\frac{p}{\rho}\right)+\frac{\mathbf{E}\times\mathbf{B}}{\mu_0}-\mathbf{v}\cdot\tau'-k\nabla T\right]+\rho h+\rho\mathbf{v}\cdot\nabla\psi, \tag{6}$$

where $\mathbf{B}$ and $\mathbf{E}$ are magnetic and electric fields, e is the internal energy, p is the pressure, $\boldsymbol{\tau}'$ is the deviatoric stress, k is the thermal conductivity (we have used Fourier's law of heat conduction), T is the temperature and h is the local heat generation. The left-hand side gives the rate of increase of internal, kinetic and magnetic energy per unit volume. The divergence on the right-hand side gives the inward flux of kinetic, internal, compressional, electromagnetic and shear energy plus the heat flowing in by conduction. The final two terms are the heat source per unit volume and work done by gravitational forces.

Integrating eq. (6) over the entire core, combining kinetic and internal energy terms and using eqs (2), (3), and the divergence theorem gives

$$\begin{aligned}\frac{d}{dt}\int\rho e\,dV+\frac{d}{dt}\int\frac{1}{2}\rho\mathbf{v}^2\,dV+\int\frac{\partial}{\partial t}\frac{\mathbf{B}^2}{2\mu_0}dV\\ =-\oint p\mathbf{v}\cdot d\mathbf{S}-\oint\frac{\mathbf{E}\times\mathbf{B}}{\mu_0}\cdot d\mathbf{S}\\ +\oint\mathbf{v}\cdot\boldsymbol{\tau}'\cdot d\mathbf{S}+\oint k\nabla T\cdot d\mathbf{S}\\ +\int\rho h\,dV+\int\rho\mathbf{v}\cdot\nabla\psi dV.\end{aligned} \tag{7}$$

The left-hand side of this equation gives the total rate of change of internal, kinetic and magnetic energy. The surface integrals on the right-hand side give the work done on the surface by pressure forces, the flux of electromagnetic energy across the boundary, the work done by surface tractions and the heat flux across the boundary. The final two volume integrals give the total heat supplied and the total work done against gravitational forces.

We now make some simplifying assumptions. The first is to average out the time fluctuations associated with the convection and dynamo process to leave integrals that describe only the slow evolution of the basic state. This averaging process has been discussed by many authors, most completely by Braginsky & Roberts (1995). They did not include the effects of thermal contraction; we include it here by averaging $\mathbf{v}$ not to zero but to $\mathbf{u}$, the radial velocity of the slow contraction. Care is needed in evaluating the averages of some of the integrals because products of fluctuating quantities do not average to the product of their averages. The second simplifying assumption is to remove effects of changes in the mantle. We remove the flux of electromagnetic energy across the core surface by taking the mantle to be an electrical insulator and the work done by shear stresses on the boundary by invoking a stress-free boundary. Gravitational energy is a property of the whole Earth: it cannot be separated into contributions from the core and mantle, for example. Changes in gravitational energy are calculated in terms of the work done by gravitational forces during the change. It is possible to integrate the work done in the core and call this the gravitational energy change of the core, but changing mantle density alters the gravitational potential in the core and thereby affects the core calculation. We neglect these mantle effects in our calculations.

The remaining terms in eq. (7) may be rearranged to give Q, the heat lost through the core–mantle boundary (CMB)

$$\begin{aligned}Q&=-\oint k\nabla T\cdot d\mathbf{S}\\ &=\int\rho h\,dV-\frac{d}{dt}\int\rho e\,dV\\ &\quad+\int\rho\mathbf{v}\cdot\nabla\psi\,dV-\oint p\mathbf{u}\cdot d\mathbf{S},\end{aligned} \tag{8}$$

where each integral is taken over the whole core and is time-averaged. Q cannot be estimated from basic state values because heat is transferred by convection in the main body of the fluid and conducted out through a surface boundary layer. We cannot therefore replace ∇T in eq. (8) by the adiabatic temperature gradient; in fact, one use of eq. (8) is to determine the superadiabatic temperature gradient in the boundary layer.

The second term represents the rate of change of internal energy. As it stands it includes the convective fluctuations, but we only require the long-term evolution. The time derivative stands outside the integral, so the rate of change may be estimated by differencing total internal energies over an interval that is long compared with the convective timescale. The only contributing changes are then those associated with the long timescale, giving

$$\frac{d}{dt}\int\rho e\,dV=\int\rho\left(\frac{\partial e}{\partial t}+\mathbf{u}\cdot\nabla e\right)dV, \tag{9}$$

where ρ and e are also basic state values. This equation simply states that the convective fluctuations can only change the internal energy through changes to the basic state. This is a general rule for time derivatives of global quantities.

The third term in eq. (8) is the work done by gravitational forces; it also contains $\mathbf{v}$ explicitly. However, it is also the rate of change of gravitational energy and its long-term average may also be estimated purely in terms of basic state variables. Consider the gravitational energy of the whole Earth. The work done by gravitational forces is then

$$\begin{aligned}\int_\infty\rho\mathbf{v}\cdot\nabla\psi\,dV&=\int_\infty\nabla\cdot(\rho\psi\mathbf{v})\,dV-\int_\infty\psi\nabla\cdot(\rho\mathbf{v})\,dV\\ &=\int_\infty\psi\frac{\partial\rho}{\partial t}\,dV.\end{aligned} \tag{10}$$

The left-hand side depends on $\mathbf{v}$ and therefore the convective fluctuations. The right-hand side does not depend on $\mathbf{v}$ explicitly, but it does so implicitly because ψ depends on ρ and therefore fluctuates with the convection. However, it is straightforward to show, using the law of gravity

$$\nabla^2\psi=-4\pi G\rho \tag{11}$$

that

$$\int_\infty\psi\frac{\partial\rho}{\partial t}\,dV=\int_\infty\rho\frac{\partial\psi}{\partial t}\,dV=\frac{1}{2}\frac{d}{dt}\int_\infty\rho\psi\,dV, \tag{12}$$

where d/dt can been taken out of the integral because it is over all space. The integral on the right-hand side is the standard formula for the gravitational energy of a self-gravitating body, which does not depend on how the mass was brought together because gravitational force is conservative. It has the form of the time derivative of a global quantity, and its long-term evolution may therefore be estimated in terms of the slow evolution of the Earth. Therefore, $\mathbf{v}$ may be replaced by $\mathbf{u}$ in the third term of eq. (8) and $\rho\nabla\psi$ by the hydrostatic pressure gradient. We extend the result to the Earth's core using the simplifying approximation of ignoring changes in the core caused by mantle changes. This also ignores the possibilities of underplating the core–mantle boundary or percolation of material from the mantle into the core.

This completes the proof that energy loss may be estimated from integrals over the basic state. All terms on the right-hand side of eq. (8) apply to a self-gravitating body in hydrostatic equilibrium. Under such conditions the change in gravitational energy is entirely taken up in work done by pressure forces during the contraction. To show this we combine the last two integrals on the right-hand side of eq. (8) with part of the change in internal energy. First, note that Reynolds' transport theorem allows the internal energy integral to be written in terms only of the slow contraction:

$$\frac{d}{dt}\int \rho e\, dV = \int \rho \frac{De}{Dt} dV,$$

where now D/Dt involves $\mathbf{u}$. Then use the thermodynamic relation

$$T ds = de - \frac{p\, d\rho}{\rho^2} \tag{13}$$

to give

$$\int \rho \frac{De}{Dt}\, dV = \int \rho T \frac{Ds}{Dt}\, dV + \int \frac{p}{\rho}\frac{D\rho}{Dt}\, dV$$
$$= \int \rho T \frac{Ds}{Dt}\, dV - \int p \nabla\cdot\mathbf{u}\, dV. \tag{14}$$

Substituting this into eq. (8) gives a contribution $\int p\nabla\cdot\mathbf{u}\, dV$. Next, change $\mathbf{v}$ to $\mathbf{u}$ in the surface integral on the right-hand side of eq. (8) and convert it to a volume integral with the divergence theorem. Finally, combine all three pressure integrals to give

$$\int p\nabla\cdot\mathbf{u}\, dV + \int \mathbf{u}\cdot\nabla p\, dV - \int \nabla\cdot(p\mathbf{u})\, dV = 0. \tag{15}$$

Entropy is a function of T and P and it changes with time in response to both cooling and the increase in pressure caused by the contraction:

$$\frac{Ds}{Dt} = \left(\frac{\partial S}{\partial T}\right)_p \frac{DT}{Dt} + \left(\frac{\partial S}{\partial p}\right)_T \frac{Dp}{Dt}. \tag{16}$$

Eq. (16) may be rewritten in terms of the standard definitions for specific heat at constant pressure, C_p, and the coefficient of thermal expansion at constant temperature, α:

$$C_p = T\left(\frac{\partial S}{\partial T}\right)_p \tag{17}$$

$$\alpha = -\rho\left(\frac{\partial S}{\partial p}\right)_T \tag{18}$$

$$= -\frac{1}{\rho}\left(\frac{\partial \rho}{\partial T}\right)_p \tag{19}$$

(by a Maxwell relation) to give

$$\rho T \frac{Ds}{Dt} = \rho C_p \frac{DT}{Dt} - \alpha T \frac{Dp}{Dt}. \tag{20}$$

The first term on the right-hand side of eq. (20) is simply the heat released by a drop in temperature at constant pressure. It includes the latent heat of freezing and some dependence on the contraction through $\mathbf{u}$ in the Lagrangian derivative. The second term gives the heating that arises from an increase in pressure. It has been called 'adiabatic' heating by some (Gubbins *et al.* 1979; Stacey & Stacey 1999), but is really heat released by an isothermal increase in pressure. We therefore call it 'pressure' heating.

Substituting from eq. (20) into eq. (8) gives our final heat balance

$$Q = \int \rho h\, dV - \int \rho C_p \frac{DT}{Dt}\, dV + \int \alpha T \frac{Dp}{Dt}\, dV. \tag{21}$$

Eq. (21) equates heat passing through the CMB to the sum of heat sources and heat released by cooling, freezing and contraction. It does not contain the magnetic field, so we cannot use it to assess the heat required to maintain the geodynamo. Physically, this is because the magnetic energy is derived from other sources (friction) and is dissipated as Ohmic heating. Mathematically, the magnetic field obeys its own energy equation, a balance between work done by the fluid against magnetic forces, Ohmic heating and the rate of change of magnetic energy.

2.3 The entropy equation

Magnetic field enters the entropy balance. The entropy equation at a point is given by

$$\rho \frac{Ds}{Dt} = \frac{\nabla\cdot(k\nabla T)}{T} + \frac{(\rho h + \Phi)}{T} \tag{22}$$

(Hewitt *et al.* 1975). Φ is the combined Ohmic and viscous heating. Integrating over the core gives the gross entropy balance. Note that the left-hand side is then in the correct form to apply Reynolds' transport theorem, and therefore the result does not depend on the convection. The integral may therefore be estimated by considering only the slow evolution of the core, and the $\mathbf{v}$ that appears implicitly in the Lagrangian derivative may be replaced with $\mathbf{u}$ and other quantities replaced with their basic state values—in particular the pressure can be taken as being hydrostatic and the temperature as adiabatic.

Integrating eq. (22) over the core gives the gross entropy balance. The first term on the right-hand side is converted using the divergence theorem

$$\int \frac{\nabla\cdot(k\nabla T)}{T}\, dV = -\frac{Q}{T_c} + \int k\left(\frac{\nabla T}{T}\right)^2 dV, \tag{23}$$

where T_c is the temperature of the CMB, assumed to be uniform. Using eq. (20) for the rate of change of entropy in the left-hand side of eq. (22) and substituting for Q from eq. (21) gives

$$\int \left(\rho h - \rho C_p \frac{DT}{Dt} + \alpha T \frac{Dp}{Dt}\right)\left(\frac{1}{T_c} - \frac{1}{T}\right) dV$$
$$= \int \frac{\Phi}{T} dV + \int k\left(\frac{\nabla T}{T}\right)^2 dV. \tag{24}$$

Eq. (24) has a simple physical interpretation. The right-hand side contains the dissipative contributions, all of which are positive and represent part of the inexorable descent of the Universe into chaos. The left-hand side contains the entropy changes arising from having heat sources and sinks at different temperatures, all multiplied by a local 'efficiency factor' $(T - T_c)/T_c$.

3 ESTIMATING INDIVIDUAL TERMS

We now need to make numerical estimates of each of the terms in eqs (21) and (24).

3.1 Radioactive heating

These are calculated assuming uniform h, because the vigorous core convection will mix any radiogenic elements uniformly. The heat is then simply

$$Q_R = \int \rho h \, dV = M_c h, \tag{25}$$

where M_c is the mass of the core. The entropy contribution contains the integral

$$I_T = \int \frac{\rho}{T} \, dV \tag{26}$$

and is

$$E_R = \int \rho h \left(\frac{1}{T_c} - \frac{1}{T} \right) dV = \left(\frac{M_c}{T_c} - I_T \right) h. \tag{27}$$

3.2 Cooling on the adiabat

The cooling term has two parts, each of which have one contribution from the volume of the fluid and one from the freezing at the inner core boundary (ICB). All terms are proportional to the cooling rate, which varies with depth in the core. A very useful approximation relates the local cooling rate at radius r to that at the CMB. The adiabatic temperature satisfies the equation

$$T_a(r) = T_c \exp\left(\int_r^{r_c} \frac{g\gamma}{\phi} dr \right) = T_i \exp\left(- \int_{r_i}^{r} \frac{g\gamma}{\phi} dr \right), \tag{28}$$

where $T_i = T(r_i)$ is the temperature of the inner core boundary, γ is Grüneissen's parameter, ϕ is the seismic parameter, g is the acceleration due to gravity and r_c is the outer core radius (Poirier 2000). The exponent will change slowly over time with cooling but the effect on T_a is negligible. Therefore,

$$\frac{1}{T}\frac{DT}{Dt} = \frac{1}{T_c}\frac{dT_c}{dt}, \tag{29}$$

which is independent of position. One may therefore take $T^{-1}DT/Dt$ out of all the integrals. Note that the Lagrangian derivative operating on T_c simply measures the drop of temperature on the CMB itself, rather than at a fixed radius. Rough estimates of the changes in g, γ and ϕ with temperature suggest that eq. (29) is accurate to better than 1 per cent.

3.3 Specific heat

Another very useful approximation is to take C_p as constant, which it is within the uncertainties of our knowledge concerning properties of core iron. The specific heat contributions to eqs (21) and (24) are then simply

$$Q_S = -\int \rho C_p \frac{DT}{Dt} \, dV = -C_p \frac{1}{T_c}\frac{dT_c}{dt} I_S, \tag{30}$$

where

$$I_S = \int \rho T \, dV \tag{31}$$

and the entropy contribution to eq. (24) is

$$E_S = -\int \rho C_p \left(\frac{1}{T_c} - \frac{1}{T} \right) \frac{DT}{Dt} \, dV$$
$$= C_p \left(M_c - \frac{I_S}{T_c} \right) \frac{1}{T_c}\frac{dT_c}{dt}. \tag{32}$$

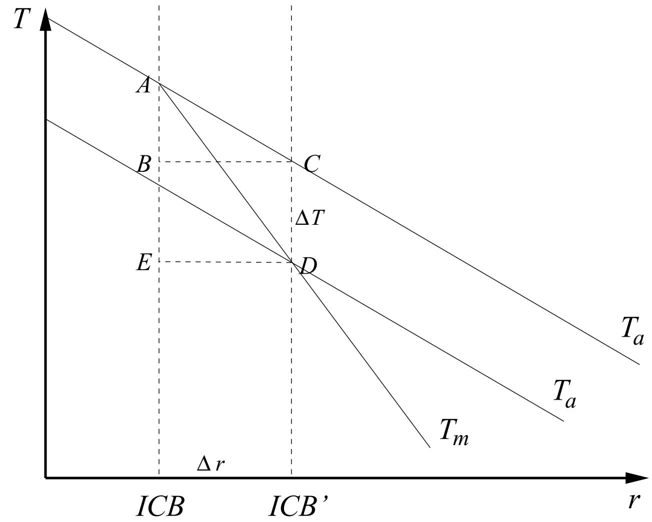

Figure 1. Inner core growth with falling temperature. Initially the inner core radius is at ICB, where the ambient adiabatic temperature T_a intersects the melting temperature T_m. The adiabatic temperature drops by $\Delta T = CD$ and the inner core radius increases by Δr to ICB$'$, the new intercept with T_m. If $'$ denotes a derivative with respect to r, then $AE = T'_m \Delta r$ and $AB = T'_a \Delta r$. $\Delta T = AE - AB$. Rearranging gives $\Delta r = \Delta T/(T'_m - T'_a)$.

3.4 Latent heat

The latent heat released depends on the rate of advance of the ICB,

$$Q_L = 4\pi r_i^2 L \rho(r_i) \frac{dr_i}{dt}. \tag{33}$$

The cooling rate at the ICB is, from eq. (29)

$$\frac{dT_i}{dt} = \frac{T_i}{T_c}\frac{dT_c}{dt}. \tag{34}$$

The ICB advances to keep the ambient temperature equal to the melting temperature of iron, T_m. Since both melting and adiabatic temperatures vary with radius, the advance depends on the difference of their gradients (Fig. 1):

$$\frac{dr_i}{dt} = -\frac{1}{(dT_m/dp - dT_a/dp)} \frac{T_i}{\rho g} \frac{1}{T_c} \frac{dT_c}{dt}. \tag{35}$$

Combining eqs (33) and (35) gives

$$Q_L = -\frac{4\pi r_i^2 L T_i}{(dT_m/dp - dT_a/dp) g} \frac{1}{T_c}\frac{dT_c}{dt}. \tag{36}$$

The entropy contribution is simply

$$E_L = -\frac{4\pi r_i^2 L (T_i - T_c)}{(dT_m/dp - dT_a/dp) T_c g} \frac{1}{T_c}\frac{dT_c}{dt}. \tag{37}$$

Mathematically, latent heat may be regarded as a specific heat singularity at $r = r_i$: when the core cools by a small amount ΔT the freezing releases latent heat concentrated at the ICB. The integrals (30) and (32) for Q_S and E_S can be made to include the latent heat by using a modified specific heat:

$$C'_p = C_p + L\delta(r - r_i)/(T'_m - T'_a). \tag{38}$$

A similar device will be used in calculating the pressure heating.

3.5 Pressure changes

Two terms in eqs (24) and (21) require knowledge of the rate of change of pressure. Contraction produces a change in hydrostatic pressure at a given radius within the Earth. Near the surface the pressure is reduced because the Earth's radius is reduced and there is less material above, but for most of the Earth, and all of the core, the pressure increases because g is larger (more mass inside radius r) and ρ is larger. The pressure change for a given change in temperature produces further compression, which in turn causes a further pressure increase. The total pressure change is found iteratively. Braginsky & Roberts (1995) gave an alternative method which uses an approximation to avoid the clumsy iteration.

Consider the effect of a small increase in density $\delta\rho$ that produces a contraction in volume. By conservation of mass, the change in radius is

$$\delta r = -\frac{\int_0^r \delta\rho(r')r'^2\, dr'}{\rho(r)r^2} \tag{39}$$

and the change in g is

$$\delta g = \int_0^r \delta\rho(r')r'^2\, dr' \frac{4\pi G}{r^2}. \tag{40}$$

The change in pressure is given by integrating the gradient of hydrostatic pressure

$$\delta p_v(r) = \int_r^a (\delta\rho g + \delta g\rho)\, dr' + \delta a\rho(a)g(a) - \delta r\rho(r)g(r). \tag{41}$$

The volume change on freezing also produces a change in the pressure. Consider the change following an increase in inner core radius $\delta r_{\rm i}$. The change in radius is

$$\delta r_{\rm f} = \frac{f r_{\rm i}^2}{r^2}\delta r_{\rm i}, \tag{42}$$

where f is the fractional volume change on freezing. The change in g is simply that due to the extra mass below radius r:

$$\delta g_{\rm f}(r) = 4\pi r_{\rm i}^2 G f \frac{\rho}{r^2}\delta r_{\rm i} \tag{43}$$

and the pressure change is simply

$$\delta p_{\rm f}(r) = \int_r^a \rho\delta g_{\rm f}\, dr'. \tag{44}$$

The rate of increase of density due to cooling alone is

$$\rho\alpha\frac{DT}{Dt} = \rho\alpha T\frac{1}{T_{\rm c}}\frac{dT_{\rm c}}{dt}. \tag{45}$$

The rate of increase of $r_{\rm i}$ is given by eq. (35) and is also proportional to the CMB cooling rate. Consider changes in a small interval of time dt. The CMB temperature will change by $\delta T_{\rm c}$, the density will change by

$$\delta\rho = -\rho\alpha T\frac{\delta T_{\rm c}}{T_{\rm c}} \tag{46}$$

and

$$\delta r_{\rm i} = -\frac{1}{(dT_{\rm m}/dp - dT_{\rm a}/dp)}\frac{T_{\rm i}}{\rho g}\frac{\delta T_{\rm c}}{T_{\rm c}} \tag{47}$$

in eqs (39)–(44) to obtain δp_v, $\delta p_{\rm f}$, δr and $\delta r_{\rm f}$.

Eqs (39)–(44) are non-linear because the density on the right-hand side depends on the pressure. We solve them by iteration. The total change in pressure $\delta p = \delta p_v + \delta p_{\rm f}$ causes a further change in density:

$$\delta\rho_p(r) = \frac{\delta p}{\phi} \tag{48}$$

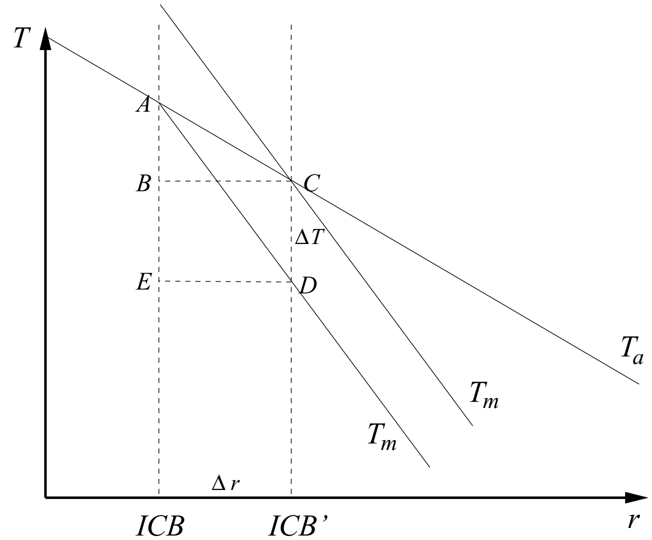

Figure 2. Inner core growth with increasing pressure. The melting point rises by $\Delta T = dT_{\rm m}/dp\Delta p$, the inner core radius increases by Δr where the new melting point curve meets the adiabat. $AE = T'_{\rm m}\Delta r$ and $AB = T'_{\rm a}\Delta r$. $\Delta T = AE - AB$, and rearranging gives $\Delta r = [dT_{\rm m}/dp/(T'_{\rm m} - T'_{\rm a})]\Delta p$.

and a further change in inner core radius because the increase in pressure elevates the melting temperature (Fig. 2):

$$\delta r_{\rm i}^p = \frac{dT_{\rm m}/dp}{dT_{\rm m}/dp - dT_{\rm a}/dp}\frac{\delta p}{\rho_{\rm i} g_{\rm i}}. \tag{49}$$

The additional changes in ρ and $r_{\rm i}$ are added on and the pressure recalculated. Iteration proceeds to convergence.

This determines δp in terms of $\delta T_{\rm c}$, and hence the rate of change of pressure with time as a numerical coefficient P_T times the cooling rate:

$$\frac{Dp}{Dt} = P_T\frac{dT_{\rm c}}{dt}. \tag{50}$$

3.6 Pressure heating

The volumetric pressure contributions to the energy and entropy equations were calculated numerically from the rate of increase of pressure:

$$Q_P = \int \alpha T P_T\, dV\frac{dT_{\rm c}}{dt} \tag{51}$$

$$E_P = \frac{Q_P}{T_{\rm c}} - \int \alpha P_T\, dV\frac{dT_{\rm c}}{dt}. \tag{52}$$

Pressure heating appears alongside specific heat everywhere in the equations, and assists in driving the dynamo in the same way as the specific heat.

The pressure changes are awkward to compute because of the iterative nature of the calculation, yet one's intuition suggests they are small. They have been treated in some detail here because of differences of opinion in the literature over the fate of the change in gravitational energy of the Earth. However, complicated numerical calculations are not the best way to eliminate an otherwise plausible physical process, and the reader may, like the authors, prefer the following more qualitative argument.

First, transform the pressure heating term Q_P by regarding p as a function of density and temperature:

$$\frac{Dp}{Dt} = \left(\frac{\partial p}{\partial \rho}\right)_T \frac{D\rho}{Dt} + \left(\frac{\partial p}{\partial T}\right)_\rho \frac{DT}{Dt} \tag{53}$$

$$= \frac{K_T}{\rho}\frac{D\rho}{Dt} + \alpha K_T \frac{DT}{Dt}, \tag{54}$$

where we have used the usual definition for K_T and the thermodynamic relation

$$\left(\frac{\partial p}{\partial T}\right)_\rho = \alpha K_T. \tag{55}$$

We neglect the difference between K_T and the bulk modulus derivable from seismology, K_S, which is of the order of $K_T \alpha\gamma T$ with $\alpha\gamma T \approx 0.05$. Transforming the first term on the right of eq. (54) with the equation of mass conservation then gives

$$Q_P = \int \alpha T \frac{Dp}{Dt}\, dV = -\int \alpha K_S T \left(\nabla \cdot \mathbf{u} - \alpha \frac{DT}{Dt}\right) dV. \tag{56}$$

Consider the two terms in parentheses on the right-hand side. The first is the dilatation rate, $\nabla \cdot \mathbf{u}$. The second is the rate of change of relative volume due to cooling, but it is subtracted from the total dilatation rate. The quantity in parentheses is therefore the rate of shrinkage caused by the increase in pressure alone.

The second term on the right-hand side of eq. (56) has the same form as the specific heat contribution Q_S in eq. (30). The ratio of the integrands is

$$\frac{\alpha^2 K_T T}{\rho C_p} \approx \alpha\gamma T \approx 0.05, \tag{57}$$

where we have again approximated K_T with K_S. This contribution to the heat supply is therefore only about 5 per cent of the specific heat. Note that it is actually subtracted: it is in fact a heat sink. The volume change due only to pressure, which itself arises only because of density changes, is probably even smaller than that due directly to the temperature (estimates for a uniform sphere give the ratio of the pressure to the temperature effect on density as $4p/3K_S \approx 0.3$). This argument leads us to believe that Q_P is a small percentage of the specific heat, within the margin of error in our knowledge of C_p.

A similar argument allows us to compare the first term on the right-hand side of eq. (56) to the work done by pressure forces in contraction, $\int p \nabla \cdot \mathbf{u}\, dV$. The ratio of the integrands in this case is

$$\frac{\alpha K_T T}{p} \approx 0.20 \tag{58}$$

so the total contribution Q_P should not exceed 20 per cent of the work done by pressure forces and is likely to be much less because our estimate included the thermal contraction. This is confirmed by detailed calculations (see Table 3 in Section 4.3).

3.7 Pressure effect on freezing

The increase in pressure elevates the melting point of iron and causes additional growth of the inner core. A change in pressure Δp causes an increase in the inner core radius (Fig. 2) given by

$$\Delta r_{\mathrm{i}} = \frac{dT_{\mathrm{m}}/dp}{T'_{\mathrm{m}} - T'_{\mathrm{a}}}\Delta p. \tag{59}$$

The heat contribution is therefore

$$Q_{PL} = \frac{4\pi r_{\mathrm{i}}^2 \rho L\, dT_{\mathrm{m}}/dp}{T'_{\mathrm{m}} - T'_{\mathrm{a}}} P_T \frac{dT_{\mathrm{c}}}{dt} \tag{60}$$

and the corresponding entropy is

$$E_{PL} = Q_{PL}\left(\frac{1}{T_{\mathrm{c}}} - \frac{1}{T_{\mathrm{i}}}\right). \tag{61}$$

Q_{PL} has the same form as the latent heat Q_{L} in eq. (36) and may be regarded simply as an enhancement to L. Replacing L in eq. (36) by

$$L' = \left(L + \frac{dT_{\mathrm{m}}}{dp} P_T\right) \tag{62}$$

gives the sum $Q_{\mathrm{L}} + Q_{PL}$.

3.8 Volume change on freezing: a thermal expansion anomaly

Müller & Häge (1979) computed the change in Earth's gravitational energy arising from the volume change on freezing. Liquid iron increases in density when it freezes, causing contraction of the whole Earth and a loss of gravitational energy. What happens to this energy? According to the calculation made by Müller & Häge (1979), over 70 per cent of it becomes available to drive the dynamo, in contradiction to Loper's (1978) estimate of 30 per cent. Like the gravitational energy released by thermal contraction, the only part of this energy that is available to drive the dynamo is the pressure heating. We now show that this pressure heating is exactly equal to the latent heat released by elevation of the melting point by the higher pressure given in eq. (60).

We treat the volume change on freezing as a thermal expansion singularity, in the same way as the latent heat was treated as a specific heat singularity. Let the fractional volume decrease on freezing be f. A drop in temperature ΔT produces a relative volume change $\int \alpha \Delta T\, dV$ from thermal contraction, and a growth of inner core radius $\Delta T/(T'_{\mathrm{m}} - T'_{\mathrm{a}})$ with consequent relative volume change $4\pi r_{\mathrm{i}}^2 f \Delta T/(T'_{\mathrm{m}} - T'_{\mathrm{a}})$. This volume change from freezing can be incorporated into the thermal expansion coefficient by redefining it as

$$\alpha' = \alpha + \frac{f\delta(r - r_{\mathrm{i}})}{T'_{\mathrm{m}} - T'_{\mathrm{a}}}. \tag{63}$$

Substituting the extra contribution into eq. (56) for Q_P gives

$$\frac{4\pi r_{\mathrm{i}}^2 f T_{\mathrm{i}}}{T'_{\mathrm{m}} - T'_{\mathrm{a}}}\frac{DP_{\mathrm{i}}}{Dt}. \tag{64}$$

The Clapeyron equation relates the volume change on freezing and latent heat to the melting point gradient. In the present notation it is

$$\frac{dT_{\mathrm{m}}}{dp} = \frac{Tf}{\rho L}. \tag{65}$$

Substituting eq. (65) into eq. (64) to eliminate f in favour of L gives

$$\frac{4\pi r_{\mathrm{i}}^2 \rho(r_{\mathrm{i}}) L}{T'_{\mathrm{m}} - T'_{\mathrm{a}}}\frac{DT_{\mathrm{i}}}{Dt}, \tag{66}$$

which is the latent heat released by the extra freezing caused by the pressure change.

This analysis shows that volume change on freezing does not contain any new energy sources for the dynamo, as claimed by Müller & Häge (1979), it merely forces the inner core to freeze faster than it would under temperature change alone, thereby releasing more latent heat.

3.9 Dissipation

The entropy gain from thermal diffusion is

$$E_k = \int k \left(\frac{\nabla T}{T}\right)^2 dV. \tag{67}$$

It is estimated using the adiabatic temperature. The range of adiabatic gradients used in this paper yield E_k in the range 2–5 × 10^8 W K^{-1}.

The entropy gain from Ohmic heating requires a model of the magnetic field and electric currents in the core

$$E_\Phi = \int \frac{\mathbf{J}^2}{\sigma T} dV. \tag{68}$$

We know the magnetic field at the core surface but not inside. This places a lower bound on E_Φ but a realistic value is much larger. A toroidal field must exist inside the core, and it could be very much larger than the observed poloidal field. Secondly, the Ohmic heating depends critically on the length-scale of the magnetic field inside the core, and if this is small the Ohmic heating will be large. Gubbins *et al.* (1979) used kinematic dynamo models, with the dipole moment scaled to that of the Earth today, We now have dynamic dynamo models to give a somewhat more realistic estimate of E_Φ, but they will still be an underestimate. The benchmark dynamo (Christensen *et al.* 1999) has a weak internal magnetic field and gives $E_\Phi \approx 2 \times 10^5$ W K^{-1}, not much more than the lower bound discussed by Gubbins *et al.* (1979). The dynamo model of Kuang & Bloxham (1997) has a more realistic magnetic field and gives $E_\Phi \approx 4 \times 10^7$ W K^{-1} (Bloxham, personal communication). Roberts *et al.* (2002) discuss the Ohmic heating in the core based on the geodynamo simulation of Glatzmaier & Roberts (1996) and a consideration of small-scale magnetic fields. They arrive at a figure of 2 TW for the Ohmic heating, which for a mean core temperature of 4500 K yields $E_\Phi = 4 \times 10^8$ W K^{-1}. This estimate is significantly larger that those in the numerical simulations because of the inclusion of small-scale fields. We consider the larger figure to be the better estimate for the core.

The viscous contribution is usually neglected because molecular viscosity is so small, but it is now widely accepted that core convection is highly turbulent and a more appropriate turbulent viscosity is six or more orders of magnitude larger. However, even with this much larger value the contribution to the dissipation entropy remains small because the kinetic energy is so much less than the magnetic energy. We should bear in mind that the viscous contribution could be significant if small-scale turbulence is much stronger than it is presently thought to be.

We assume a total dissipation entropy of 10^9 W K^{-1}—tantamount to assuming E_Φ and E_k are comparable in magnitude. This could be an overestimate by as much as a factor of 5, or an underestimate. The principal results are proportional to this quantity, so it is trivial to assess their sensitivity to changes in the assumed value.

3.10 Two simple equations

The energy and entropy equations (21) and (24) give two simple equations that must be satisfied in order to maintain the geodynamo:

$$Q = Q_\mathrm{R} + Q_\mathrm{S} + Q_\mathrm{L} + Q_P + Q_{PL} = \mathcal{A}h + \mathcal{B}\frac{dT_\mathrm{c}}{dt} \tag{69}$$

$$E_k + E_\Phi = E_\mathrm{R} + E_\mathrm{S} + E_\mathrm{L} + E_P + E_{PL} = \mathcal{C}h + \mathcal{D}\frac{dT_\mathrm{c}}{dt}, \tag{70}$$

where each term on the right-hand side is defined as an integral over core properties multiplied by the internal heating h (for Q_R and E_R) or the CMB cooling rate DT_c/Dt. Q is defined in eq. (8); Q_R in eq. (25), Q_S in eq. (30), Q_L in eq. (36), Q_P in eq. (51), Q_{PL} in eq. (60); and E_R in eq. (27), E_S in eq. (32), E_L in eq. (37), E_P in eq. (51), E_{PL} in eq. (61); E_k in eq. (67) and E_Φ in eq. (68).

We use eq. (70) to determine combinations of h and DT_c/Dt that give the left-hand side, which is fixed at 10^9 W K^{-1}. We compute two separate cases, one with no cooling and one with no internal heating; it is then a simple matter to assess the results for a combination of the two.

We use the energy eq. (69) to compute the heat flux across the CMB, Q, once the heat source and cooling rates are established. Eq. (35) gives the rate of growth of the inner core in terms of the cooling rate.

4 CALCULATIONS AND RESULTS

The coefficients in eqs (69) and (70) are integrals over core properties: temperature, density, compressibility, thermal expansivity, specific and latent heats, thermal and electrical conductivities, and the melting temperature and its derivative with respect to pressure. With the exception of the conductivities, for which we use common values quoted in the literature, we could obtain all of these properties from first-principles (FP) calculations on iron. However, it is more realistic and accurate to use the results of seismology wherever possible. We use model PREM (Dziewonski & Anderson 1981).

Every term depends on the temperature within the core, which is derived by integrating the adiabatic gradient from the ICB to the CMB. The starting temperature is determined from the melting point of the iron alloy in the outer core. We consider a pure iron core, and use the properties of iron with one exception: we use a lower ICB temperature to allow for depression of the melting point by impurities in the outer core (amounting to about 800 K).

4.1 First-principles calculations for the properties of pure iron

The thermodynamic properties of pure iron have been extracted from the Helmholtz free energy, which has been calculated as a function of volume and temperature using *first-principles* simulations. FP simulations have been done on systems containing up to ≈100 Fe atoms, in which the nuclei are treated as classical particles, and the electrons are treated fully quantum mechanically. The motion of the ions is adiabatically separated from that of the electrons, and this approximation is justified by the large difference of mass between Fe ions and electrons. The quantum mechanics calculations for the electrons are based on density functional theory (DFT) (Hohenberg & Kohn 1964; Kohn & Sham 1965), which is a formulation of quantum mechanics alternative to the Schrödinger equation. DFT is exact in principle, though to solve the problem in practice one needs a fundamental approximation for the so-called *exchange-correlation* energy. We have used the generalized gradient approximation (Wang & Perdew 1991), which has proved to give results in good agreement with the experiment for the structural and vibrational properties of Fe (Stixrude *et al.* 1994; Söderlind *et al.* 1996; Vočadlo *et al.* 1997; Alfè *et al.* 2000a).

The key quantity for the calculation of the thermodynamic properties of Fe is the Helmholtz free energy

$$F = -k_\mathrm{B} T \ln\left\{\frac{1}{N!\Lambda^{3N}} \times \int_V d\mathbf{R}_1 \cdots d\mathbf{R}_N \exp\left[-\beta U(\mathbf{R}_1, \ldots \mathbf{R}_N; T)\right]\right\}, \tag{71}$$

where N is the number of particles in the system, $\Lambda = h/(2\pi M k_B T)^{1/2}$ is the thermal wavelength, with M being the nuclear mass, h Planck's constant, k_B Boltzmann's constant and $\beta = 1/k_B T$. The multidimensional integral extends over the total volume of the system V.

A direct calculation of F using the equation above is impossible, since it would involve knowledge of the potential energy $U(\mathbf{R}_1, \dots \mathbf{R}_N; T)$ for all possible positions of the N atoms in the system. We use instead the technique known as *thermodynamic integration* (see e.g. Frenkel & Smit 1996), as developed in earlier papers (Sugino & Car 1995; de Wijs *et al.* 1998; Alfè *et al.* 1999a). This is a general scheme to compute the free energy difference $F_1 - F_0$ between two systems with potential energies of U_1 and U_0, respectively. The basic idea is that $F_1 - F_0$ represents the reversible work done on continuously and isothermally switching the energy function from U_0 to U_1. To do this switching, a continuously variable energy function U_λ is defined as

$$U_\lambda = (1 - \lambda)U_0 + \lambda U_1, \tag{72}$$

so that the energy goes from U_0 to U_1 as λ goes from 0 to 1. In classical statistical mechanics, the work done in an infinitesimal change $d\lambda$ is

$$dF = \langle dU_\lambda/d\lambda\rangle_\lambda\, d\lambda = \langle U_1 - U_0\rangle_\lambda \lambda, \tag{73}$$

where $\langle \cdot \rangle_\lambda$ represents the thermal average evaluated for the system governed by U_λ. It follows that

$$F_1 - F_0 = \int_0^1 d\lambda \langle U_1 - U_0\rangle_\lambda. \tag{74}$$

In practice, this formula can be applied by calculating $\langle U_1 - U_0\rangle_\lambda$ for a suitable set of λ values and performing the integration numerically. The average $\langle U_1 - U_0\rangle_\lambda$ is evaluated by sampling over configuration space. In our case the sampling is performed using FP molecular dynamics.

The Helmholtz free energy of the system is then $F = F_0 + (F - F_0)$, so if one knows the free energy of the reference system F_0 one has a complete scheme to calculate the free energy of the *ab initio* system F. It is important to stress that the choice of the reference system does not affect the final answer for F, though it affects the efficiency of the calculations. This can be understood by analysing the quantity $\langle U_1 - U_0\rangle_\lambda$, which is the thermal average of the potential energy difference between the two systems. If this difference has large fluctuations then one would need very long simulations to calculate the average value to a sufficient statistical accuracy. Moreover, for an unwise choice of U_0 the quantity $\langle U_1 - U_0\rangle_\lambda$ may depend strongly on λ so that one would need a large number of calculations at different λ values in order to compute the integral in eq. (74) with sufficient accuracy. It is crucial then to find a good reference system, where good means a system for which the fluctuations of $U_1 - U_0$ are as small as possible.

For liquid Fe we found that an exceptionally good reference system is just a simple sum of inverse power potentials:

$$U_{\mathrm{IP}} = \frac{1}{2}\sum_{I \neq J} \phi(|\mathbf{R}_I - \mathbf{R}_J|), \tag{75}$$

where $\phi(r) = B/r^\alpha$, with B and α being adjusted to minimize the fluctuations of the difference between U_{IP} and the *ab initio* energy. The free energy of an inverse power potential was calculated using thermodynamic integration in which the reference potential was the Lennard-Jones potential, for which the free energy has been computed and reported in Johnson *et al.* (1993). As a consistency check we have also performed the thermodynamic integration using the perfect gas as a reference system, and we have found the same results, within the precision limit of 0.5 kJ mol^{-1}.

For iron we performed the calculations at 18 different thermodynamic states spanning the conditions of density and temperature of the outer core. The calculated Helmholtz free energies are fitted to a simple functional form of volume and temperature. All the thermodynamic quantities of interest are then obtained by appropriate differentiation of F. The specific heat at constant pressure C_p is

$$C_p = C_V + \frac{VT}{K_T}\left[\left(\frac{\partial p}{\partial T}\right)_V\right]^2, \tag{76}$$

where

$$p = -\left(\frac{\partial F}{\partial V}\right)_T \tag{77}$$

$$K_T = -V\left(\frac{\partial p}{\partial V}\right)_T \tag{78}$$

and

$$C_V = -\left(\frac{\partial^2 F}{\partial T^2}\right)_V. \tag{79}$$

The expansion coefficient is

$$\alpha = \frac{1}{V}\left(\frac{\partial V}{\partial T}\right)_p = \frac{1}{K_T}\left(\frac{\partial p}{\partial T}\right)_V \tag{80}$$

and the Grüneisen parameter is

$$\gamma = V\left(\frac{\partial p}{\partial E}\right)_V = V\left(\frac{\partial p}{\partial T}\right)_V \Big/ \left(\frac{\partial E}{\partial T}\right)_V, \tag{81}$$

where E is the internal energy

$$E = F - TS = F + \left(\frac{\partial F}{\partial T}\right)_V T. \tag{82}$$

We estimate an error of $\approx$1.5 kJ mol^{-1} in F, which propagates in the derived quantities. Since the free energy is fitted to a polynomial form, every differentiation of F lowers the order of the polynomial by one, with the result of worsening the quality of the corresponding thermodynamic quantities. We estimate an error of a few per cent in γ, α and C_p.

The resulting parameters are given under column CORE in Table 1. C_p and γ are independent of pressure to within the accuracy of the calculation. α decreases strongly with pressure as shown in Fig. 3. Most of these parameters affect the solution for heat generation and cooling rate rather transparently, making it easy

Table 1. Comparison of numerical values between two previous calculations and new values. Where the quantity varies with pressure the range is given, pressure at ICB first. Variation of α for model CORE is shown in Fig. 3. Units: $\alpha \times 10^{-5}$ K^{-1}; C_p in J kg^{-1} K^{-1}; $L \times 10^6$ J kg^{-1}; k in W m^{-1} K^{-1}; T_{i} in K; temperature gradients in K GPa^{-1}.

Quantity	GMJ79	LPL97	CORE	LOWT
α	0.55–1.0	1.35	1.02–1.95	1.02–1.95
C_p	700	860	715	715
γ	0.9–1.2	1.6–1.2	1.5	1.5
L	1.0	0.62	0.75	0.75
k	50	60	60	60
T_{i}	4070	5070	5500	4500
dT_M/dP	–	9.0	9.0	9.0
$(\partial T/\partial P)_S$	2.8	6.9	5.9	5.9
Difference	1.4–10.0	2.1	3.1	3.1

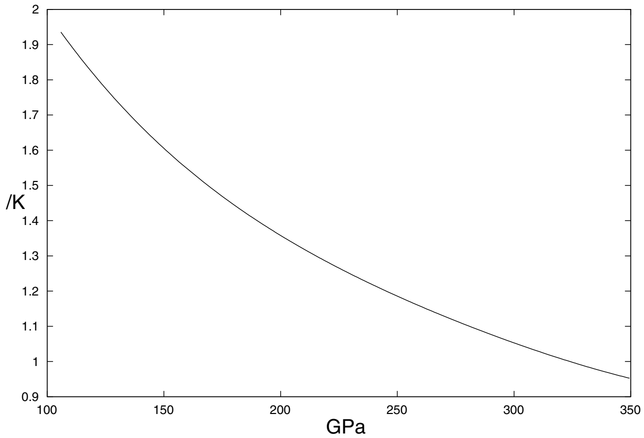

Figure 3. Thermal expansion coefficient for model CORE in units of 10^{-5} K^{-1}.

to assess the effect of errors on the final solution without further calculation, except for the temperature, which enters most of the integrals, sometimes along with its gradient. We therefore make some comparisons of different temperature models in the next section to assess the possible uncertainties.

4.2 Comparison models for the temperature

The core properties used in three studies are compared in Table 1: CORE is the present model, based on FP calculations modified by reducing the temperature by 800 K to account for the lower melting point of the mixture. LPL97 is from Labrosse *et al.* (1997) and GMJ79 refers to Gubbins *et al.* (1979). The only substantive differences are in α and γ and their variation with pressure: these affect the radial variation of the adiabatic gradient. Model LOWT is included to assess the effect of a lower core temperature. It has $\gamma = 1.5$ and $T_\mathrm{i} = 4500$ K, 1000 K colder than for CORE.

The adiabatic temperature is computed by integrating eq. (28). The calculations are relatively insensitive to uncertainties and variations in α unless we use a form of eq. (28) that contains α explicitly, as Labrosse *et al.* (1997) have done. They effectively assumed $\alpha\rho/C_p$ to be independent of pressure in order to obtain an adiabatic gradient with a simple analytical form. This is equivalent to using eq. (28) with γ proportional to ϕ/ρ, because of the thermodynamic definition

$$\gamma = \frac{\alpha\phi}{C_p}. \tag{83}$$

Labrosse *et al.* (1997) therefore have γ increasing with pressure; the other models have either γ nearly constant or decreasing with pressure (Table 1).

The near-constant γ of model CORE is consistent with the recent study of Anderson & Ahrens (1994), who obtain $\gamma \propto \rho^{-0.2}$. Constant γ has an interesting consequence. From the thermodynamic relation (e.g. Gubbins & Masters 1979)

$$\left(\frac{\partial\gamma}{\partial P}\right)_\mathrm{S} = -\frac{\gamma}{K_\mathrm{S}}\left[1+\gamma-\left(\frac{\partial K_s}{\partial P}\right)_\mathrm{S}+\delta_\mathrm{S}\right], \tag{84}$$

where the adiabatic Anderson–Grüneissen parameter is

$$\delta_\mathrm{S} = -\frac{1}{\alpha K_\mathrm{S}}\left(\frac{\partial K_s}{\partial T}\right)_P \tag{85}$$

and since $K_\mathrm{S} = \rho v^2{}_P$ in the core we have

$$\delta_\mathrm{S} = 1 - \frac{1}{\alpha v_p^2}\left(\frac{\partial v_P^2}{\partial T}\right)_P \tag{86}$$

and eq. (84) becomes

$$\left(\frac{\partial\gamma}{\partial P}\right)_\mathrm{S} = -\frac{\gamma}{K_\mathrm{S}}\left[2+\gamma-\left(\frac{\partial K_s}{\partial P}\right)_\mathrm{S}-\frac{1}{\alpha v_P^2}\left(\frac{\partial v_P^2}{\partial T}\right)_P\right]. \tag{87}$$

The first three terms in the brackets on the right-hand side sum to near zero for most estimates of core parameters, including model CORE, for which

$$\gamma \approx 1.5 \tag{88}$$

$$\left(\frac{\partial K_s}{\partial P}\right)_\mathrm{S} \approx 3.5. \tag{89}$$

Eq. (87) then gives

$$\left(\frac{\partial v_P^2}{\partial T}\right)_P \approx 0. \tag{90}$$

The P-wave velocity does not vary with temperature. This is a surprising result: the high pressure almost completely inhibits the normal temperature dependence of the P-wave speed.

Gubbins *et al.* (1979) considered a γ satisfying $(\partial\phi/\partial T)_P \approx -2000$ m^2 s^{-2} K^{-1}

$$\frac{1}{\alpha v_P^2}\left(\frac{\partial v_P^2}{\partial T}\right)_P \approx -2. \tag{91}$$

Using this estimate in eq. (87) gives, after some manipulation,

$$\left(\frac{\partial\gamma}{\partial\rho}\right)_\mathrm{S} = -\frac{2\gamma}{\rho}, \tag{92}$$

which integrates to

$$\gamma = \frac{A}{\rho^2}, \tag{93}$$

where A is a constant of integration. This is consistent with an earlier analysis of shock wave data by Jeanloz (1979).

In this paper we include two models with γ based on eq. (93), partly to provide an extreme case and partly to provide some comparison with the previous work of Gubbins *et al.* (1979). This gives four different choices of γ. A fifth model has a lower ICB temperature.

(1) Model CORE with its own adiabatic temperature gradient, corresponding to $\gamma \approx 1.5$

(2) Model LPL97 using parameters of Labrosse *et al.* (1997).

(3) Model CMB, as CORE but with γ given by eq. (93) and A chosen so that $\gamma = 1.5$ at the CMB.

(4) Model ICB, as CORE but with γ given by eq. (93) and A chosen so that $\gamma = 1.5$ at the ICB. This has a substantially higher γ overall.

(5) Model LOWT, as CORE but with $T_\mathrm{i} = 4500$ K.

Models (3) and (4) are similar to those in Gubbins *et al.* (1979) and, with (2), give a comparison with previously published work.

The corresponding adiabatic temperatures are shown in Fig. 4. The differences are small, the largest being the effect of lower melting temperatures in LPL97 and LOWT and steeper gradient caused by the larger average γ of model ICB. Their effect on the energy calculations will be shown in the next section to be small, vindicating the simple approximation made by Labrosse *et al.* (1997).

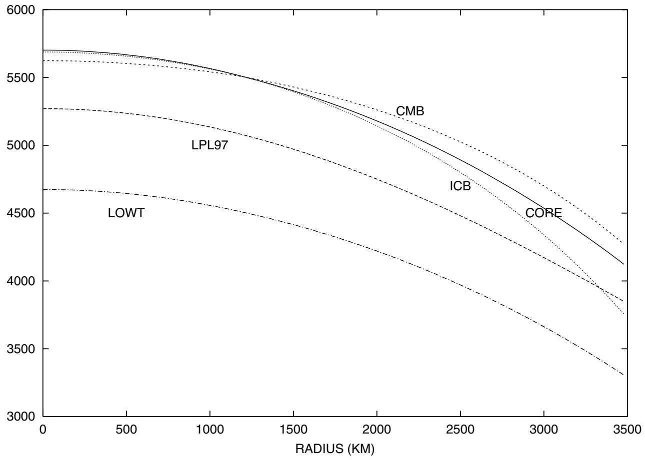

Figure 4. Adiabatic temperature gradients for the different models.

Table 2. Radioactive heating models. h is in units of 10^{-12} W kg^{-1}, Q in TW, E in M W K^{-1}. Q_k is the heat conducted down the adiabat at the CMB.

Model	h	Q_R	Q_k	E_Φ	E_k
CORE	**16**	**31.4**	**8.6**	**740**	**260**
LPL97	17	32.2	6.4	792	208
CMB	18	34.4	9.6	767	233
ICB	11	20.9	12.7	568	532
LOWT	12	23.6	7.4	700	300

4.3 Results

The results for uniform radioactive heating are given in Table 2. E_k and Q_k, the heat conducted at the CMB down the adiabat, depend only on the model parameters and not the cooling rate or radioactive heating. All of the models involve very high heat flux across the CMB—between 50 and 75 per cent of the Earth's surface heat flux, and correspondingly large amounts of radiogenic material. Most would consider these quantities too large to fit with any reasonable thermal history of the whole Earth. We discuss this point in the next section.

ICB is the only model giving significantly different results. These arise because this model has a substantially larger γ throughout the outer core (1.5–2.26), which produces a larger adiabatic gradient. It is interesting to note that this model requires the least radioactive heating (Q_R) despite losing the most heat by conduction down the adiabat (Q_k). The steep adiabat produces a large temperature difference between the ICB and the CMB, making the heat engine more efficient. The greater efficiency overcomes the extra heat lost by conduction. This result illustrates the danger of only considering heat conducted down the adiabat at the CMB when estimating the power required to drive the dynamo.

Results for cooling are given in Table 3. The rate of increase of the inner core radius is calculated using eq. (35); the inner core age is computed by dividing the volume of the inner core by the calculated volumetric freezing rate, $4\pi r_i^2 dr_i/dt$. This assumes a constant rate of loss of latent heat and gives only a very rough estimate of inner core age. A constant cooling rate would give older inner core ages. More accurate estimates require a proper thermal history that includes the mantle, which ultimately controls the cooling rate of the core. Thermal histories will be included in future studies.

Again the heat fluxes are high, although somewhat smaller than the radioactive heating models in Table 2 because the latent heat (and to some extent the heat released by cooling) appears deeper in the core at a higher temperature, and therefore the entropies are larger. This can be seen from Table 3 by comparing the relative contributions of Q_L (47 per cent) and E_L (62 per cent): the entropy contribution is bigger because the latent heat is released at the ICB, the hottest part of the outer core.

Pressure heating is small, as expected, amounting to only a few per cent of the total heat passing across the CMB. However, the increase in pressure caused by contraction does produce a significant acceleration of the growth of the inner core. The column per cent p in Table 3 gives the proportion of dr_i/dt that comes from the pressure increase rather than temperature decrease. This was predicted by Müller & Häge (1979), but it is not, as they supposed, a new source of energy: it is merely a faster rate of release of latent heat.

Cooling produces a contraction of 5–10 km in 1 Gyr for these models. The density and pressure both increase by 1–2 per cent in the same time. The pressure change amounts to a maximum of about 6 GPa in the outer core; mantle cooling produces only 30 MPa. The extra inner core growth caused by pressure depends on the melting gradient. For model CORE this is 9 K GPa^{-1}; 6 GPa would elevate the melting temperature by 54 K and advance the ICB. The advance is 54 divided by the difference between the melting and adiabatic gradients, which for this model is 0.14 K km^{-1}: almost 400 km.

The last model in Table 3 is the same as CORE except that the latent heat has been set to zero in order to give an estimate of the cooling rate required to drive the dynamo in the distant past before the inner core was formed. The cooling rate and heat flux is much greater than for other models, as expected.

5 DISCUSSION

There is now impressive agreement on the properties of iron at core temperatures and pressures. Temperature gradients are rather uncertain but the results shown in Tables 2 and 3 appear to be rather insensitive to them. Model ICB has a very large value of γ and must be considered extreme. It confirms the assertion made by Gubbins *et al.* (1979) that only γ, not its pressure derivative $d\gamma/dp$, influences

Table 3. Results for cooling. 'Per cent p' gives the percentage inner core growth caused by pressure changes; the rest comes from cooling. Units are: dT/dt in K Gyr^{-1}; dr_i/dt in km Gyr^{-1}; IC age in Myr.

Model	dT_c/dt	dr_i/dt	Per cent p	IC age	Q_L	Q_{PL}	Q_S	Q_P	Q	E_L	$E+PL$	E_S	E_P
CORE	**168**	**1602**	**18**	**254**	**9.8**	**1.8**	**8.6**	**0.3**	**20.5**	**595**	**109**	**280**	**17**
LPL97	187	1833	20	222	8.3	1.6	11.3	0.3	21.6	623	102	358	18
CMB	271	1526	13	267	9.8	1.2	13.7	0.4	25.1	513	65	404	18
ICB	95	1185	22	344	7.0	1.6	5.2	0.2	14.0	594	132	258	17
LOWT	147	1127	16	361	7.0	1.1	7.6	0.2	15.9	566	89	330	15
NOIC	565	–	–	–	–	28.8	1.1		28.8	–	943		57

the thermodynamic estimates seriously. Model CORE yields very similar results to LPL97, although the inner core age is much less here because we have not considered compositional convection and we have imposed a fixed entropy requirement. Henceforth we shall use only model CORE for the discussion.

Model CORE requires too much heat. The Earth's surface heat flux is usually taken to be about 45 TW. For radioactive heating CORE requires 70 per cent of all the surface heat to originate in the core. Most authors expect no more than 25 per cent to come from the core, and many would prefer less than 10 per cent. The source of all this heat is an additional problem: $h = 16 \times 10^{-12}$ W kg^{-1} translates into 0.2 μW m^{-3}, or about 30 per cent of current estimates of radioactive heating in the continental crust, where most of the Earth's radiogenic elements are thought to be concentrated.

Cooling (Table 3) gives slightly lower heat requirements, but still 46 per cent of Earth's surface heat flux. The rapid cooling rate requires a concomitant cooling of the mantle, which also contributes to the total heat budget. Taking a mean temperature drop of 100 K Gyr^{-1} in the mantle, half that at the CMB, and a mean specific heat of 1200 J kg^{-1} K^{-1}, gives an additional 16 TW of heat from cooling the mantle. Secular cooling then accounts for 81 per cent of the heat budget, leaving very little for radioactivity anywhere in the Earth. Rapid cooling also freezes the inner core quickly: it seems improbable that the inner core formed less than 300 Ma.

All the recent published models of core evolution have a young inner core—typically 1–2 Ga. There is therefore a need for some mechanism to generate the magnetic field before the inner core formed. Compositional convection cannot operate without an inner core because the light material is released by freezing; this leaves only thermal convection. Model NOIC gives a rough estimate of the heat required to drive the dynamo without an inner core. The cooling rate is very high because there is no latent heat: if the inner core is only 1 Gyr old, we would have to drive the dynamo for 3 Gyr with this mechanism, invoking a drop in temperature of 1700 K plus the drop in the last 1 Gyr. This very high cooling rate implies very high temperatures and a partially molten lower mantle in the distant past.

We must clearly reduce the heat requirements for the model to work. The most important deficiency is the lack of compositional convection, which is included in the companion paper. However, it is worth exploring how the heat flow can be reduced by adjusting the model parameters before altogether dismissing thermal convection as the main driving force for the geodynamo. A combination of radioactive heating and cooling would alleviate the problem of freezing the inner core too quickly but would exacerbate the problem of high heat flow into the mantle. Similarly, raising the specific heat estimate, or the latent heat, would slow the freezing of the inner core but leave the heat flow problem. Changing the melting point gradient would also change the rate of freezing of the inner core and drop the cooling rate for the same heat flux, but the inner core would freeze even faster. Reducing k reduces E_k but it also reduces the electrical conductivity because they are coupled through the Wiedemann–Franz law, and this increases E_Φ. Reducing the adiabatic gradient reduces the heat conducted away, but it also reduces the dynamo efficiency (as shown by the results for model ICB).

A sure way to reduce the heat flux substantially is to reduce the entropy requirement from 1000 MW K^{-1}. E_k gives something of a lower bound; choosing $E = E_k$ reduces all the heat fluxes in proportion, along with h and cooling rates. For model CORE $E_k = 260$ W K^{-1}, so everything is reduced by a factor of 0.26 (and the inner core age in increased by 1/0.26). The inner core age rises to 1.0 Ga, the cooling rate falls to 44 K Gyr^{-1}, and the total heat flux to 5.3 TW, or 12 per cent of the total heat budget. For radioactive heating the total heat flux is 8.2 TW (28 per cent).

The total heat flux in both cases is less than the heat conducted down the adiabat ($Q_k = 8.6$ TW, Table 2), a contradiction of the assumptions of the model. This contradiction can only be resolved by allowing the temperature gradient to become subadiabatic in the outer part of the core. For the cooling model, some convection will exist deep in the core, where the adiabatic gradient is not so steep. For radioactive heating this may not be the case, because the conduction temperature for a uniform distribution of heat sources is similar to the adiabat: the core may become subadiabatic everywhere.

To maintain convection throughout the core we must have $Q \geq Q_k$, or 8.6 TW. This value of Q is 19 per cent of the Earth's surface heat flux and yields $E = 420$ MW K^{-1}: 160 for E_Φ and 260 for E_k, assuming viscous contributions are negligible. This is enough to drive a dynamo with magnetic fields of the right magnitude and length-scales comparable to those in the current generation of numerical simulations, but not any significant small-scale magnetic fields. The cooling rate is also reduced by a factor of 0.398 to 70 K Gyr^{-1} and the inner core age increased to 638 Myr.

Setting $Q = Q_k$ in model NOIC gives a cooling rate of 331 K Gyr^{-1}, still extraordinarily high. Setting $E = E_k$ for the same model gives 147 K Gyr^{-1}. Reducing the cooling rate still further will shut off all convection in the core. Heat is then carried entirely by conduction. It is worth exploring this extreme limit for model NOIC because the necessary cooling rate is quite large.

Convection ceases when the conduction gradient becomes smaller in magnitude than the adiabatic gradient. The conduction gradient satisfies the heat conduction equation subject to suitable boundary and initial conditions. Boundary conditions present no problem: the solution must be regular at the origin and the temperature is specified at the CMB. Initial conditions are another matter: they depend on the early thermal state of the core, which is unknown. The conduction profile (its variation with radius) will in general change with time unless it is a natural decay mode. The slowest decaying mode gives a conduction profile that can usefully be compared with the adiabat; it represents the ultimate temperature profile after all transients have died away.

The decay mode has the form

$$T = \frac{T_c}{j_0(\beta r_c)} j_0(\beta r) \exp(-qt), \tag{94}$$

where j_0 is a spherical Bessel function ($j_0(x) = \sin x/x$),

$$\beta = \sqrt{q/\kappa}, \tag{95}$$

q is the decay rate determined by the cooling rate:

$$xq = -\frac{1}{T_c}\frac{dT_c}{dt} \tag{96}$$

and κ is the thermal diffusivity

$$\kappa = \frac{k}{\rho C_p}. \tag{97}$$

Choosing numerical values from the tables in this paper and a cooling rate of 145 K Gyr^{-1} gives a conduction profile that is just subadiabatic throughout the core. 150 K Gyr^{-1} gives a superadiabatic gradient out to radius 1300 km. These values are very close to that for $E = E_k$ because the decay mode profile is very similar to the adiabat throughout the core. A very rapid cooling rate is therefore required to maintain any form of convection in an entirely liquid core.

6 CONCLUSIONS

(1) Core properties are now sufficiently well known for calculations of power requirements for the geodynamo to be reliable. *First-principles* calculations on liquid iron are in broad agreement with other estimates of core properties, at least in terms of the demands of the calculations in this paper.

(2) The change in Earth's gravitational energy caused by thermal contraction and volume change on freezing is significant (4–10 TW in these models) but most of it does not contribute to driving the dynamo. The pressure increase associated with thermal contraction causes some heating, adding about 2 per cent to the overall heat flux. The change in gravitational energy associated with the change in volume on freezing is, by the Clapeyron equation, equal to the latent heat released by freezing caused by the rise in melting temperature associated with the increased pressure—it is not a new source of energy for the dynamo.

(3) Thermal convection is thermodynamically inefficient in generating magnetic fields, and all models require a large heat flux to cross the core–mantle boundary. An extreme model, in which convection is just maintained throughout the core requires 12.5 TW for radioactive heating and 8.6 TW for cooling. More realistic models require four times this value.

(4) If the geodynamo is driven by cooling the inner core may be less than 1 Gyr old, the preferred age being less than 300 Ma. Maintaining a magnetic field before the inner core formed requires very high cooling rates. Without an inner core all the heat could be carried by conduction for cooling rates up to 145 K Gyr^{-1}, which is rather higher than most thermal histories assume. The geodynamo therefore places a very powerful constraint on the Earth's early thermal history, one that should be useful in eliminating many speculative models.

Further geophysical discussion is postponed until Paper II, which includes compositional convection.

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