Appendix A. Balance equations

We use a combined numerical strategy for modelling convection by solidstate creep in the Earth's mantle as well as partial melting in some of the upper regions of the mantle, processes that lead to the segregation and formation of the precursors of continental crustal material as well as mixing within the remaining mantle. We solve differential equations relating to infinite Prandtl-number convection using a three-dimensional finite-element spherical-shell method that ensures the conservation of mass, momentum, and energy. The mass balance

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = 0 \tag{A.1}$$

with an anelastic-liquid approximation simplifies to

$$\nabla \cdot \vec{v} = -\frac{1}{\rho} \vec{v} \cdot \nabla \rho \tag{A.2}$$

where ρ is density, t is time, and \vec{v} is velocity.

The conservation of momentum can be written as

$$\rho\left(\frac{\partial \vec{v}}{\partial t} + \vec{v} \cdot \nabla \vec{v}\right) = -\nabla P + \rho \vec{g} + \frac{\partial}{\partial x_k} \tau_{ik} \tag{A.3}$$

where P is pressure, \vec{g} is acceleration due to gravity, and τ_{ik} is the deviatoric stress tensor. Spherical symmetry is modelled using $\vec{g} = -g\vec{e_r}$ and the hydrostatic pressure gradient is defined as

$$-\frac{\partial P}{\partial r} = \rho g \tag{A.4}$$

By definition, $K_S = -V\left(\frac{\partial P}{\partial V}\right)_S$ and $\frac{V}{V_0} = \frac{\rho_0}{\rho}$, where K_S is the adiabatic bulk modulus, V is volume, S is entropy, and r is the radial distance from the Earth's centre. Hence,

$$K_S = \rho \left(\frac{\partial P}{\partial \rho}\right)_S = \rho \left(\frac{\partial P}{\partial r}\right)_S \left(\frac{\partial r}{\partial \rho}\right)_S \tag{A.5}$$

Substituting Eq. (A.4) into Eq. (A.5) yields

$$\left(\frac{\partial\rho}{\partial r}\right)_{S} = \frac{-\rho^{2}g}{K_{S}} \tag{A.6}$$

If horizontal spatial variations in ρ are ignored, Eqs. (A.2) and (A.6) yield

$$\nabla \cdot \vec{v} = -\frac{1}{\rho} \vec{v} \cdot \nabla \rho \cong -\frac{1}{\rho} v_r \frac{\partial \rho}{\partial r} = \frac{\rho g v_r}{K_S}$$
(A.7)

It is well known that

$$K_S = \frac{c_p}{c_v} K_T = (1 + \alpha \gamma_{th} T) K_T \tag{A.8}$$

where K_T is the isothermal bulk modulus, c_p is specific heat at a constant pressure, c_v is specific heat at a constant volume, α is the coefficient of thermal expansion, γ_{th} is the thermodynamic Grüneisen parameter, and T is the absolute temperature.

This means that eq. (A.3) can be rewritten as

$$\rho \frac{dv_i}{dt} = \rho g_i + \frac{\partial \sigma_{ki}}{\partial x_k} \tag{A.9}$$

This in turn means that the energy balance can be expressed as follows

$$\rho \frac{du}{dt} + \frac{\partial q_i}{\partial x_i} = Q + \sigma_{ik} \dot{\varepsilon}_{ik} \tag{A.10}$$

where u is specific internal energy, Q is heat generation rate per unit volume, and v_i , g_i , q_i , x_i , σ_{ik} , and $\dot{\varepsilon}_{ik}$ are velocity, gravity acceleration, heat flow density, location vector, stress tensor, and strain-rate tensor components, respectively.

Another formulation of Eq. (A.10) is

$$\rho \left[\frac{\partial}{\partial t} + \vec{v} \cdot \nabla \right] u = \nabla \cdot (k \nabla T) + Q - P \nabla \cdot \vec{v} + 2W_D \tag{A.11}$$

where

$$2W_D = \sigma_{ik} \dot{\varepsilon}_{ik} + P \bigtriangledown \cdot \vec{v} \tag{A.12}$$

and

$$q_k = -k \frac{\partial T}{\partial x_k} \tag{A.13}$$

with k indicating thermal conductivity. Using

$$du = T \ ds - P \ dv \tag{A.14}$$

and

$$du = T\left(\frac{\partial s}{\partial T}\right)_P dT + T\left(\frac{\partial s}{\partial P}\right)_T dP - Pdv \tag{A.15}$$

eliminates specific internal energy (u) in Eq. (A.11), yielding the following equation

$$\rho c_p \frac{dT}{dt} = \nabla \cdot (k \nabla T) + Q + \alpha T \frac{dP}{dt} + 2W_D \tag{A.16}$$

as

$$c_p = T\left(\frac{\partial s}{\partial T}\right)_P$$
 and $\left(\frac{\partial s}{\partial P}\right)_T = -\left(\frac{\partial v}{\partial T}\right)_P = -v\alpha$ (A.17)

where s represents specific entropy, v specific volume, c_p specific heat at a constant pressure, and α the coefficient of thermal expansion.

A less well-known version of the energy balance can be deduced, as Eq. (A.11) is equivalent to

$$\rho\left(\frac{du}{dt} + P\frac{dv}{dt}\right) = \tau_{ik}\frac{\partial v_i}{\partial x_k} + \nabla \cdot (k \nabla T) + Q \qquad (A.18)$$

because of Eq. (A.2) and $\frac{1}{\rho} = v$. Inserting Eq. (A.14) into Eq. (A.18) yields

$$\rho T \frac{ds}{dt} = \tau_{ik} \frac{\partial v_i}{\partial x_k} + \frac{\partial}{\partial x_j} \left(k \frac{\partial}{\partial x_j} T \right) + Q \tag{A.19}$$

However,

$$ds = \left(\frac{\partial s}{\partial T}\right)_{v} dT + \left(\frac{\partial s}{\partial v}\right)_{T} dv \tag{A.20}$$

and

$$\left(\frac{\partial s}{\partial T}\right)_v = \frac{c_v}{T}, \qquad \left(\frac{\partial s}{\partial v}\right)_T = \alpha K_T$$
 (A.21)

suggests that

$$Tds = c_v dT + \alpha K_T T d\left(\frac{1}{\rho}\right) \tag{A.22}$$

or

$$Tds = c_v dT - \frac{c_v \gamma T}{\rho} d\rho \tag{A.23}$$

where

$$\gamma_{th} = \frac{\alpha K_T}{c_v \rho} \tag{A.24}$$

indicates the thermodynamic Grüneisen parameter.

Inserting Eq. (A.23) into Eq. (A.19) yields

$$\rho c_v \frac{dT}{dt} - c_v \gamma T \frac{d\rho}{dt} = \tau_{ik} \frac{\partial v_i}{\partial x_k} + \frac{\partial}{\partial x_j} \left(k \frac{\partial}{\partial x_j} T \right) + Q \qquad (A.25)$$

with Eqs. (A.1) and (A.25) yielding

$$\rho c_v \frac{dT}{dt} = -\rho c_v \gamma T \frac{\partial v_j}{\partial x_j} + \tau_{ik} \frac{\partial v_i}{\partial x_k} + \frac{\partial}{\partial x_j} \left(k \frac{\partial}{\partial x_j} T \right) + Q \qquad (A.26)$$

or

$$\frac{\partial T}{\partial t} = -v_j \frac{\partial}{\partial x_j} T - \gamma T \frac{\partial v_j}{\partial x_j} + \frac{1}{\rho c_v} \left[\tau_{ik} \frac{\partial v_i}{\partial x_k} + \frac{\partial}{\partial x_j} \left(k \frac{\partial}{\partial x_j} T \right) + Q \right] \quad (A.27)$$

or

$$\frac{\partial T}{\partial t} = -\frac{\partial (Tv_j)}{\partial x_j} - (\gamma - 1)T\frac{\partial v_j}{\partial x_j} + \frac{1}{\rho c_v} \left[\tau_{ik}\frac{\partial v_i}{\partial x_k} + \frac{\partial}{\partial x_j}\left(k\frac{\partial}{\partial x_j}T\right) + Q\right]$$
(A.28)

This is an alternative formula for energy conservation. Although c_v appears in Eq. (A.28), the latter expression is equivalent to Eq. (A.16), which uses c_p . The deviatoric stress tensor can be expressed by

$$\tau_{ik} = \eta \left(\frac{\partial v_i}{\partial x_k} + \frac{\partial v_k}{\partial x_i} - \frac{2}{3} \frac{\partial v_j}{\partial x_j} \delta_{ik} \right)$$
(A.29)

in Eqs. (A.3) and (A.28), where η denotes viscosity.

As an *equation of state* we use

$$\rho = \rho_r \left[1 - \alpha (T - T_r) + K_T^{-1} (P - P_r) + \sum_{k=1}^2 \Gamma_k \Delta \rho_k / \rho_r \right]$$
(A.30)

where the index r refers to the adiabatic reference state, $\Delta \rho_k / \rho_r$ or f_{ak} denotes the non-dimensional density jump for the kth mineral phase transition, and Γ_k is a measure of the relative fraction of the heavier phase, where $\Gamma_k = \frac{1}{2} \left(1 + \tanh \frac{\pi_k}{d_k} \right)$ with $\pi_k = P - P_{0k} - \gamma_k T$ describing excess pressure π_k . The quantity P_{0k} is the transition pressure for the vanishing temperature T. A non-dimensional transition width is denoted by d_k , with γ_k representing the Clausius–Clapeyron slope for the kth phase transition. Γ_k and π_k were introduced by Richter (1973) and Christensen and Yuen (1985),

with the presence of very high Prandtl numbers meaning that the left-hand side of Eq. (A.3) vanishes. As such, we use the following version of the equation of conservation of momentum:

$$0 = -\frac{\partial}{\partial x_i}(P - P_r) + (\rho - \rho_r)g_i(r) + \frac{\partial}{\partial x_k}\tau_{ik}$$
(A.31)

The final version of the conservation of mass equation is

$$0 = \frac{\partial}{\partial x_j} \rho v_j, \tag{A.32}$$

which stems from Eq. (A.2). Equations (A.28), (A.30), (A.31) and (A.32) are a system of six scalar equations that can be used to determine six scalar unknown functions, namely T, ρ , P, and the three components of v_i .

References

References

- Christensen, U. R., Yuen, D. A., 1985. Layered convection induced by phase transitions. Journal of Geophysical Research 90, 10291–10300.
- Richter, F. M., 1973. Finite amplitude convection through a phase boundary. Geophysical Journal of the Royal Astronomical Society 35, 265–276.