Appendix A. Balance equations

We use a combined numerical strategy for modelling convection by solid-state 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

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = 0 \quad (A.1)
\]

with an anelastic-liquid approximation simplifies to

\[
\nabla \cdot \vec{v} = -\frac{1}{\rho} \vec{v} \cdot \nabla \rho \quad (A.2)
\]

where \( \rho \) is density, \( t \) is time, and \( \vec{v} \) is velocity.

The conservation of momentum can be written as

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

where \( P \) is pressure, \( \vec{g} \) is acceleration due to gravity, and \( \tau_{ik} \) is the deviatoric stress tensor. Spherical symmetry is modelled using \( \vec{g} = -g \vec{e}_r \) and the hydrostatic pressure gradient is defined as

\[
-\frac{\partial P}{\partial r} = \rho g \quad (A.4)
\]

By definition, \( K_S = -V \left( \frac{\partial P}{\partial V} \right)_S \) and \( \frac{\rho}{\rho_0} = \frac{V}{V_0} \), 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,

\[
K_S = \rho \left( \frac{\partial P}{\partial \rho} \right)_S = \rho \left( \frac{\partial P}{\partial r} \right)_S \left( \frac{\partial r}{\partial \rho} \right)_S \quad (A.5)
\]

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

\[
\left( \frac{\partial \rho}{\partial r} \right)_S = -\rho^2 g \frac{1}{K_S} \quad (A.6)
\]
If horizontal spatial variations in $\rho$ are ignored, Eqs. (A.2) and (A.6) yield

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

It is well known that

$$K_S = \frac{c_p}{c_v} K_T = (1 + \alpha \gamma_{th} T) K_T$$  (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, $\alpha$ is the coefficient of thermal expansion, $\gamma_{th}$ is the thermodynamic Grüneisen parameter, and $T$ is the absolute temperature.

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

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

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

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

where $u$ is specific internal energy, $Q$ is heat generation rate per unit volume, and $v_i$, $g_i$, $q_i$, $x_i$, $\sigma_{ik}$, 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

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

where

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

and

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

with $k$ indicating thermal conductivity. Using

$$du = T \, ds - P \, dv$$  (A.14)
and

\[ du = T \left( \frac{\partial s}{\partial T} \right)_P dT + T \left( \frac{\partial s}{\partial P} \right)_T dP - P dv \]  \hspace{1cm} (A.15)

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

\[ \rho c_p \frac{dT}{dt} = \nabla \cdot (k \nabla T) + Q + \alpha T \frac{dP}{dt} + 2W_D \]  \hspace{1cm} (A.16)

as

\[ c_p = T \left( \frac{\partial s}{\partial T} \right)_P \text{ and } \left( \frac{\partial s}{\partial P} \right)_T = - \left( \frac{\partial v}{\partial T} \right)_P = -\alpha \]  \hspace{1cm} (A.17)

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

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

\[ \rho \left( \frac{du}{dt} + P \frac{dv}{dt} \right) = \tau_{ik} \frac{\partial v_i}{\partial x_k} + \nabla \cdot (k \nabla T) + Q \]  \hspace{1cm} (A.18)

because of Eq. (A.2) and \(\frac{1}{\rho} = v\).

Inserting Eq. (A.14) into Eq. (A.18) yields

\[ \rho T \frac{ds}{dt} = \tau_{ik} \frac{\partial v_i}{\partial x_k} + \frac{\partial}{\partial x_j} \left( k \frac{\partial T}{\partial x_j} \right) + Q \]  \hspace{1cm} (A.19)

However,

\[ ds = \left( \frac{\partial s}{\partial T} \right)_v dT + \left( \frac{\partial s}{\partial v} \right)_T dv \]  \hspace{1cm} (A.20)
and
\[
\left( \frac{\partial s}{\partial T} \right)_v = \frac{c_v}{T}, \quad \left( \frac{\partial s}{\partial v} \right)_T = \alpha K_T
\]  
(A.21)
suggests that
\[
T ds = c_v dT + \alpha K_T T d\left( \frac{1}{\rho} \right)
\]  
(A.22)
or
\[
T ds = c_v dT - \frac{c_v \gamma T}{\rho} d\rho
\]  
(A.23)
where
\[
\gamma_{\text{th}} = \frac{\alpha K_T}{c_v \rho}
\]  
(A.24)
indicates the thermodynamic Gr"uneisen parameter.
Inserting Eq. (A.23) into Eq. (A.19) yields
\[
\rho c_v \frac{dT}{dt} - c_v \gamma T \frac{d\rho}{dt} = \tau_{ik} \frac{\partial v_i}{\partial x_k} + \frac{\partial}{\partial x_j} \left( k \frac{\partial}{\partial x_j} T \right) + Q
\]  
(A.25)
with Eqs. (A.1) and (A.25) yielding
\[
\rho c_v \frac{dT}{dt} = -\rho c_v \gamma T \frac{\partial v_i}{\partial x_j} + \tau_{ik} \frac{\partial v_i}{\partial x_k} + \frac{\partial}{\partial x_j} \left( k \frac{\partial}{\partial x_j} T \right) + Q
\]  
(A.26)
or
\[
\frac{\partial T}{\partial t} = -v_j \frac{\partial}{\partial x_j} T - \gamma T \frac{\partial v_j}{\partial x_j} + \frac{1}{\rho c_v} \left[ \tau_{ik} \frac{\partial v_i}{\partial x_k} + \frac{\partial}{\partial x_j} \left( k \frac{\partial}{\partial x_j} T \right) + Q \right]
\]  
(A.27)
or
\[
\frac{\partial T}{\partial t} = -\frac{\partial(T v_j)}{\partial x_j} - (\gamma - 1) T \frac{\partial v_j}{\partial x_j} + \frac{1}{\rho c_v} \left[ \tau_{ik} \frac{\partial v_i}{\partial x_k} + \frac{\partial}{\partial x_j} \left( k \frac{\partial}{\partial x_j} T \right) + Q \right]
\]  
(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
\[
\tau_{ik} = \eta \left( \frac{\partial v_i}{\partial x_k} + \frac{\partial v_k}{\partial x_i} - \frac{2}{3} \delta_{ik} \frac{\partial v_j}{\partial x_j} \right)
\]  
(A.29)
in Eqs. (A.3) and (A.28), where \(\eta\) 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 $k$th mineral phase transition, and $\Gamma_k$ is a measure of the relative fraction of the heavier phase, where

$$
\Gamma_k = \frac{1}{2} \left( 1 + \tanh \pi_k d_k \right)
$$

with $\pi_k = P - P_{0k} - \gamma_k T$ describing excess pressure $\pi_k$. The quantity $P_{0k}$ is the transition pressure for the vanishing temperature $T$. A non-dimensional transition width is denoted by $d_k$, with $\gamma_k$ representing the Clausius–Clapeyron slope for the $k$th phase transition. $\Gamma_k$ and $\pi_k$ 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:

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

(A.31)

The final version of the conservation of mass equation is

$$
0 = \frac{\partial}{\partial x_j} \rho v_j,
$$

(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 $T$, $\rho$, $P$, and the three components of $v_i$.

References

References
