Influence of heterogeneous thermal conductivity on the long-term evolution of the lower mantle thermochemical structure: implications for primordial reservoirs

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Abstract. The long-term evolution of the mantle is simulated using 2D spherical annulus geometry to examine the effect of heterogeneous thermal conductivity on the stability of reservoirs of primordial material. In numerical models, mantle conductivity is often emulated using purely depth-dependent profiles (taking on values between 3 and 9 $\mathrm{Wm^{-1}K^{-1}}$). This approach is meant to synthesize the mean conductivities of mantle materials at their respective conditions in-situ. However, because conductivity depends also on temperature and composition, the effects of these dependencies in mantle conductivity is masked. This issue is significant because dynamically evolving temperature and composition introduce lateral variations in conductivity, especially in the deep-mantle. Minimum and maximum variations in conductivity are due to the temperatures of plumes and slabs, respectively, while depth- dependence directly controls the amplitude of the conductivity (and its variations) across the mantle depth. Our simulations allow assessing the consequences of these variations on mantle dynamics, in combination with the reduction of thermochemical pile conductivity due to its expected enrichment in iron, which has so far not been well examined. The mean conductivity ratio from bottom-to-top indicates the relative competition between the decreasing effect with increasing temperature and the increasing effect with increasing depth. We find that, when depth- dependence is stronger than temperature- dependence, a mean conductivity ratio > 2 will result in long-lived primordial reservoirs. Specifically, for the mean conductivity profile to be comparable to the conductivity often assumed in numerical models, the depth- dependent ratio must be at least 9 times the surface conductivity. When the conductivity profile is underestimated, the imparted thermal buoyancy (from heat-producing element, HPE, enrichment) destabilizes the reservoirs and influences core-mantle boundary (CMB) coverage configuration and the onset of dense material entrainment. The composition- dependence of conductivity only plays a minor role that behaves similarly to a small conductivity reduction due to temperature. Nevertheless, this effect may be amplified when depth- dependence is increased. For the cases we examine, when the lowermost mantle's mean conductivity is greater than the surface conductivity, reservoirs can remain stable for very long periods of time, comparable to the age of the Earth.

1 Introduction

Tomographic studies of Earth's lower mantle revealed the presence of two large low velocity provinces (LLVPs) that overlie the core-mantle boundary (CMB). They are located below the Pacific ocean and Africa with a combined coverage of up to 30% of the CMB and vertical extents as high as 1200 km (Garnero et al., 2016). These anomalous regions have been characterized by either purely thermal (Davies et al., 2012) or combined thermal and chemical (e.g., Trampert et al., 2004) effects (the latter case being aptly referred to as thermochemical piles). Piles may further affect plume generation (e.g., Tan et al., 2011; Heyn et al., 2020) and core-to-mantle heat flow (e.g., Deschamps & Hsieh, 2019). Furthermore, plumes sourced from deep mantle reservoirs may provide a mechanism to explain the diverse chemistry observed in ocean island basalts (Deschamps et al., 2011). In light of this fact, while there are two end-member views on their origin (and chemical composition), a primordial layer (composed of anomalously dense material) or a growing layer (composed of mid-ocean ridge basalt), in this study we adopt the former.

Piles' unique chemical composition determines physical properties most importantly density, viscosity, and enrichment in HPEs that affect their long-term stability (e.g., Li et al., 2014, 2018, 2019; Gülcher et al., 2020; Citron et a., 2020). In numerical simulations, underestimating their density and viscosity contrasts with respect to the ambient mantle can result in overestimating the entrainment of dense material. An important property that influences mantle dynamics is thermal conductivity. In the studies investigating density or viscosity variations, radially defined conductivity profiles synthesized and emulated the mean contributions from either (or all of) temperature, pressure (and hence, depth), and chemical composition. However, thermal conductivity can vary greatly with temperature, pressure, and composition, which, introduces heterogeneous heat transfer through spatially extended regions of the mantle. Thus, by the nature of primordial reservoirs (i.e., having anomalous chemical composition at high temperature and pressure conditions) these dependencies will also influence their evolution.

Measured and estimated thermal conductivities of minerals are determined at variable temperature and pressure conditions relevant to regions of the mantle at shallow and great depths. In addition, aggregate compositions with variable fractions of mineral concentrations and elemental inclusions influence the mantle conductivities at depth. Thus, studies that investigate pressure effects (at fixed temperature) (e.g., Ohta et al., 2012; Dalton et al., 2013; Goncharov et al., 2015; Hsieh et al., 2017, 2018) or thermal effects (at fixed pressure) (e.g., Kanamori et al., 1968; Katsura, 1997; Hofmeister, 1999; Manthilake et al., 2011; Zhang et al., 2019) often include measurements on mineral samples with additional elemental impurities. Compared to pure magnesium end-members of mantle minerals, inclusion of other elements (e.g., iron or aluminium), into an aggregate sample can reduce thermal conductivity substantially (e.g., Ohta et al., 2012; Hsieh et al., 2017, 2018). Enrichment of a mantle aggregate in iron or aluminium-bearing minerals greatly reduce its total conductivity, as might be the case for LLVPs (Deschamps & Hsieh, 2019). In numerical models, this effect can be emulated by parametrizing a percentage reduction with the primordial composition field. Li et al. (2022) showed that composition-dependence of conductivity can raise the topography of thermochemical piles.

Estimates of thermal conductivity at high temperature and high pressure are available, but, Geballe et al. (2020) point out that calculations of thermal conductivity for bridgmanite, for example, can differ by a factor of 10 between different studies

(Haigis et al., 2012; Dekura et al., 2013; Ammann et al., 2014; Tang et al., 2014; Stackhouse et al., 2015). In addition, laboratory measurements for pyrolite at both high temperature and pressure are still relatively new (e.g., $5.9^{+4.0}_{-2.3}$ $\mathrm{Wm^{-1}K^{-1}}$ at 124 GPa and 2000 to 3000 K (Geballe et al., 2020)).

In general, measurements performed on mantle minerals have shown that thermal conductivity increases with increasing pressure. At a fixed temperature (e.g., often at room temperature $\sim 300\mathrm{K}$), measurements of thermal conductivity increases with an approximately linear trend. As the temperature fixed to a greater value, conductivity values are decreased but, the linear increase in conductivity with pressure is still maintained, even if adiabatic corrections to temperature are taken into account. Enrichment of lower mantle minerals (bridgmanite and ferropericlase) in iron greatly reduce the zero- pressure reference value and the slope of thermal conductivity (e.g., Deschamps & Hsieh, 2019). Thermal conductivities taken at room temperature and CMB pressures fall between 10 and 35 $\mathrm{Wm^{-1}K^{-1}}$ for iron-bearing bridgmanite and between 35 and 60 $\mathrm{Wm^{-1}K^{-1}}$ for iron-bearing ferropericlase (Deschamps & Hsieh, 2019). If we consider thermal conductivities in this range for the lowermost mantle, we should expect that heat-exchange in that region should be more efficient. The hot primordial reservoirs and the core could be cooled by downwelling currents and subducted slabs. However, this effect will be curbed by temperature dependence.

The thermal conductivities decrease with an increasing temperature and follow a relationship proportional to T^{-n}. The exponent n controls the temperature dependence and its value is dependent on the mechanism controlling lattice heat transport. Experimental data (e.g., Klemens, 1960; Xu et al., 2004; Dalton et al., 2013) suggest that n is typically between 0.5 for (Fe,Al)-bearing minerals (three-phonon scattering at low phonon frequency) and 1.0 for $\mathrm{MgSiO_3}$ (anharmonic three-phonon scattering). Values below $n = 0.5$ are possible which suggests that mantle minerals may be weakly temperature dependent. Manthilake et al. (2011) found $n \sim 0.2$ for Fe-bearing bridgmanite and periclase. However, these measurements were made relative to a reference temperature of 700 K and pressure of 8 GPa for periclase and 26 GPa for perovskite. Furthermore, different n values may be obtained when the parametrization of thermal conductivity has additional functional temperature dependences (Hofmeister (1999) found $n = 0.33$ for silicates and 0.9 for MgO), or if density dependence is substituted for pressure dependence (Manthilake et al., 2011). For a typical temperature dependence $n = 0.5$ and a reference temperature of 300 K, a lowermost mantle temperature of 3000 K will result in a $\sim 70\%$ reduction in conductivity. A reduction of this magnitude is quite large even for a moderate temperature dependence. Therefore, the effect of temperature may play a significant role in making the lowermost mantle very poor at transferring heat. Depending on the interactions between cool subducting slabs, primordial reservoirs enriched in HPEs may become more thermally buoyant if they cannot evacuate heat.

Temperature and depth variations in conductivity had been considered previously for Boussinesq or extended Boussinesq fluid simulations. Utilizing Hofmeister (1999)'s lattice conductivity formulation in an isoviscous Boussinesq fluid, several effects were observed: temperature increases in the lower mantle (Dubuffet et al., 1999), a stabilizing effect on mantle flow, which manifests in thick and stable plumes (Dubuffet & Yuen, 2000), and the rapid thermal assimilation of cold downwelling slabs (Dubuffet et al., 2000). Yanagawa et al. (2005) examined the effects of a purely temperature dependent conductivity in conjunction with a strongly temperature dependent viscosity and observed a cooler, thinner, upper thermal boundary layer when compared to a constant conductivity. More recently, Tosi et al. (2013) parametrized a temperature and pressure dependent thermal conductivity (and thermal expansivity) derived from mineral physics data. They observed a strong increase in bulk mantle

temperature, which suppresses bottom thermal boundary layer instabilities and causes mantle flow to be driven by instabilities at the upper thermal boundary. Li et al. (2022) examined the effect of thermal conductivity in simulations featuring a compressible fluid and thermochemical piles, but conductivity changes with temperature were not included. In addition to lateral variations in temperature related to the flow, a compressible fluid introduces an adiabatic temperature increase with depth. For an adiabatic temperature gradients in the lower mantle between 0.2 to 0.4 Kkm^{-1}, temperature will increase by approximately 600 K from the 660-transition to the core-mantle boundary (Katsura, 2022). Given the strength of thermal conductivity's dependence on temperature, a comparable adiabatic temperature increase in the lowermost mantle is not an insignificant factor to neglect in primordial reservoir's total conductivity. Neglecting compressibility may result in an overestimation of thermal conductivity, thus, changing the dynamics and evolution of primordial reservoirs.

In this study, we examine the effect of temperature-, depth-, and composition- dependent conductivity on the stability of thermochemical piles. First, we isolate the effect of purely depth- dependent thermal conductivity to understand the dynamics of primordial reservoirs under different lowermost mantle conductivity conditions. Next, we introduce the effect of temperature- and composition- dependence to examine how the heating conditions in conjunction with depth- dependence affect pile evolution. We conclude by examining the effect of a fully heterogeneous conductivity (featuring depth- dependence based on mantle minerals) on the evolution of primordial reservoirs.

2 Methods

2.1 General physical properties

We model compressible thermochemical mantle convection using the finite volume code StagYY (Tackley, 2008). Each calculation is performed in a 2D spherical annulus domain, which emulates convection in a variable-thickness slice of a spherical shell centred at the equator (Hernlund & Tackley, 2008). The reference state characterizing compressible convection is based on the calculations presented in Tackley (1998). The parameters defining this reference state are listed in the Table S1 and illustrated in Figure S1 of the Supplement.

Thermochemical reservoirs are modelled with a dense primordial material origin. An initial dense layer occupies the bottom 160 km of the lower mantle, corresponding to a volume fraction of approximately 3%. The buoyancy ratio, B, defines the density contrast between regular and primordial materials. We prescribe a value of 0.23, which corresponds to a density contrast of 95 kgm^{-3} near the surface and 152 kgm^{-3} near the CMB. The mantle is basally heated and is also internally heated by heat-producing elements (HPEs) and we prescribe a non-dimensional heating rate, $H = 20$, which corresponds to a dimensional heating rate of 5.44×10^{-12} Wkg^{-1}. We assume primordial material is enriched in HPEs and has a rate up to an order of magnitude greater than regular mantle material. The initial temperature field is based on an adiabatic temperature profile of 2000 K with surface and core-mantle boundary layer thicknesses of approximately 30 km. Random temperature perturbations with an amplitude of 125 K are uniformly distributed throughout the domain. The surface and core-mantle boundary temperatures are defined at 300 K and 3440 K, respectively. Mantle viscosity featuring depth-, temperature-, and composition- dependence

is modelled using an Arrhenius formulation. A yield stress of 290 MPa is imposed at the surface so that the development of a
stagnant-lid is avoided. Viscosity is truncated so that nondimensional viscosity values do not exceed 10^5 or fall below 10^{-3} of
the reference viscosity.

We model a phase change between upper and lower mantle materials but neglect the phase change from perovskite (pv) to
post-perovskite (ppv) at the bottom of the mantle. The effects of the pv-ppv transition properties on the stability and structure
of primordial reservoirs have been investigated previously by Li et al. (2015). There are many controlling parameters for the
pv-ppv transition including the temperature of the CMB, the viscosity contrast between pv and ppv, and the viscosity contrast
between ppv and primordial material that can affect the stability of piles. For instance, weak ppv (i.e., low viscosity contrast
between pv and ppv) and a low T_{CMB} (i.e., $T_{CMB} \sim 3350$ K) can result in entrainment of primordial reservoirs. Because of
the model setup we consider in our study, the inclusion of a pv-ppv transition may result in the entrainment of a dense pri-
mordial reservoir. Thus, the pv-ppv phase transition will mask the effect of thermal conductivity on the stability of primordial
reservoirs that we are examining.

2.2 Thermal conductivity

Heterogeneous conductivity is emulated using a non-dimensional parametrized model that characterizes variations result-
ing from non-dimensional depth, $\tilde{d} = d/D$, where the depth, d, has length scale defined by the mantle thickness, D; non-
dimensional temperature, $\tilde{T} = T/\Delta T_S$, where the temperature, T, is scaled by the super-adiabatic temperature difference,
ΔT_S; and composition, C; as separate functions. Thermal conductivity is non-dimensionalized with its surface value k_S,
which is here fixed to $3\,\mathrm{Wm^{-1}K^{-1}}$. The total conductivity is a product of each individual functional dependence. In this study,
we first consider two different depth- dependencies. First, a linear depth- dependence given by

$$\tilde{k}_D(\tilde{d}) = 1 + (K_D - 1)\tilde{d} \tag{1}$$

to explicitly examine the effect of bottom-to-top conductivity ratio. This conductivity ratio is controlled by the parameter, K_D,
so that the non-dimensional depth- dependent conductivity takes on values between 1 and K_D.

Next, we consider depth- dependence based on conductivity measurements of minerals in the upper and lower mantles.
Conductivity values in the lower mantle were based on a parametrization of conductivity profiles (defined in Deschamps
& Hsieh (2019)) for a 80%-bridgmanite (Bm) and 20%-ferropericlase (Fp) mixture. Measurements for bridgmanite were
presented by Hsieh et al. (2017) and for ferropericlase by Hsieh et al. (2018). The conductivity profile in the upper mantle
is defined by a quadratic curve that smoothly connects the surface conductivity to the conductivity profile of Bm-Fp at the
660-km transition. We find that there is good agreement between the modelled conductivity profile and the measurements of
dry and wet olivine presented by Chang et al. (2017). The total conductivity profile is defined piecewise and continuous at the

660-km transition ($\tilde{d}_{ULM} = 0.22837$) and is given by

155 $$\tilde{k}_D(\tilde{d}) = \begin{cases} \frac{3.0}{k_S}\left(1 + 15.66\tilde{d} - 16.38\tilde{d}^2\right); & \tilde{d} < \tilde{d}_{ULM} \quad \text{(Upper mantle)} \\ \frac{5.33}{k_S}\left(1 + 4.98\tilde{d} - 0.81\tilde{d}^2\right); & \tilde{d} \geq \tilde{d}_{ULM} \quad \text{(Lower mantle)} \end{cases} \tag{2}$$

The bottom-to-top conductivity ratio is 9.185 and this depth- dependence is referred to as K_{DH} in this study. Compared with the linear $K_D = 10$ depth- profile, the quadratic depth- dependence is slightly raised near the transition zone and slightly lowered near the CMB. Depth- dependent conductivity profiles are illustrated in Figure 1.
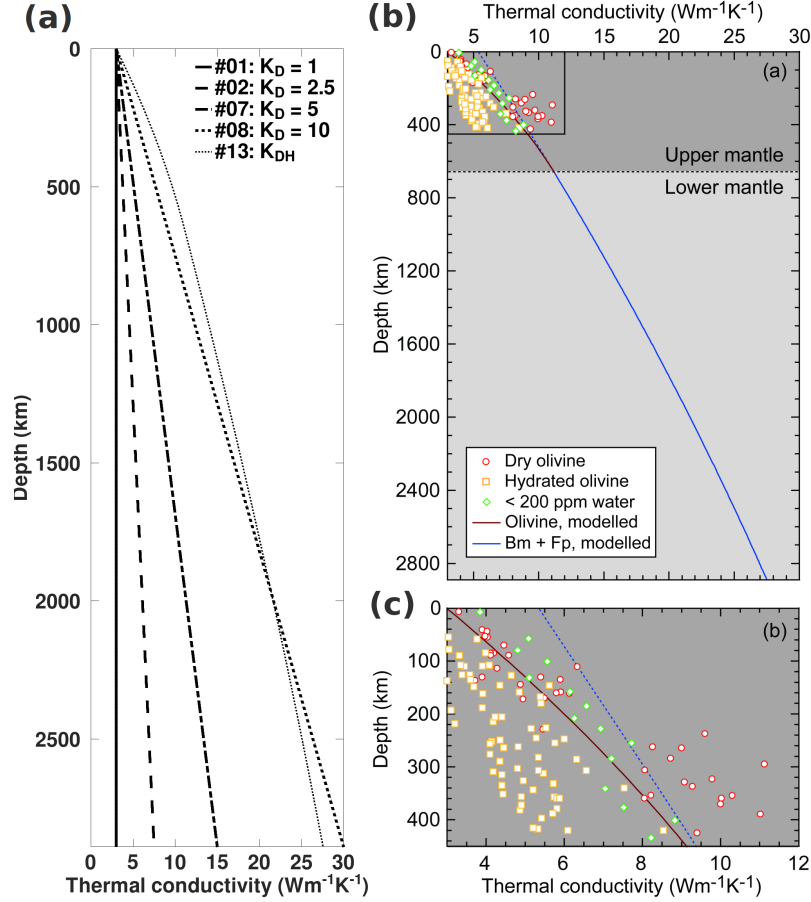
Figure 1. (a) Radial profiles for different depth- dependent conductivity functions characterized by different K_D values. (b) Conductivity measurements for upper and lower mantle materials. Olivine data points are from Chang et al. (2017) and the modelled Bm+Fp conductivity profile is based on data presented in Hsieh et al. (2017) and Hsieh et al. (2018). (c) Magnification of conductivity profile in the upper mantle.

Temperature- dependence is given by

160 $$\tilde{k}_T(\tilde{T}) = \left(\frac{(T_{surf}/\Delta T_S)}{\tilde{T}}\right)^n, \tag{3}$$

which always results in lower thermal conductivity. The super-adiabatic temperature difference, ΔT_S, is set to 2500 K. Higher values of n indicate higher sensitivity to (and thus greater reduction with) increasing temperature. In this study, we consider n values of 0.5 and 0.8. The theoretical lower limit for n is 0.5, for materials that are enriched in iron, and a value of 0.8 is representative of oxides (e.g., Klemens, 1960; Xu et al., 2004). When n is 0.0, temperature- dependence is switched off and only the remaining dependences are considered.

Composition- dependence is given by

$$\tilde{k}_C(C) = 1 + (K_C - 1)C \tag{4}$$

where K_C is the reduction factor for composition- dependence. For the primordial material considered in this study we consider corrections of 0.8 and 0.5 (corresponding to 20% and 50% conductivity reduction, respectively). When K_C is 1.0, compositional correction is switched off. Finally, the total conductivity is given by

$$k(d, T, C) = k_S \times \tilde{k}_D(d) \times \tilde{k}_T(T) \times \tilde{k}_C(C). \tag{5}$$
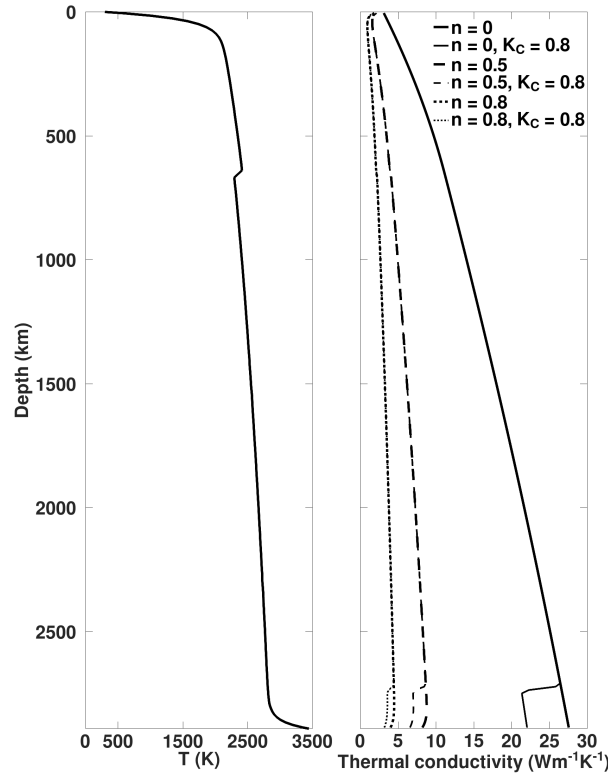
Figure 2. Initial temperature profile (left panel) and sample conductivity profiles (right panel) for cases featuring K_{DH}.

Figure 2 shows the initial temperature (left panel) and conductivity profiles (right panel) that correspond to models featuring a depth- dependence (K_{DH}) based on conductivity measurements of upper and lower mantle minerals. Different combinations of temperature- and composition- dependence are presented to show the degree of conductivity reduction resulting from these dependencies. The purely depth- dependent model ($n = 0$) has a conductivity of 27.6 $\mathrm{Wm^{-1}K^{-1}}$ at the CMB. For the T_{CMB} we consider (e.g., 3440 K), the conductivity at the CMB will be reduced by approximately 70% and 86% for $n = 0.5$ and 0.8 leading to conductivities of 8.1 and 3.9 $\mathrm{Wm^{-1}K^{-1}}$, respectively. For thermochemical material at that depth, a 20% reduction suggests conductivities of 22.0, 6.5, and 3.1 $\mathrm{Wm^{-1}K^{-1}}$ for $n = 0, 0.5$ and 0.8, respectively. Note that because the piles are enriched in HPEs, their conductivities will eventually be much lower.

The governing equation for conservation of energy given by

$$\bar{\rho} C_P \frac{DT}{Dt} = -\mathrm{Di}_{surf}\bar{\alpha}\bar{\rho}T v_Z + \nabla \cdot (k\nabla T) + \bar{\rho}H + \frac{\mathrm{Di}_{surf}}{Ra}\Phi \tag{6}$$

and may be used to briefly outline where heterogeneous conductivity affects the dynamics. The physical parameters in this equation include the reference density, $\bar{\rho}$; the reference heat capacity, $\bar{C_P}$; the reference thermal expansivity, $\bar{\alpha}$; the vertical velocity, v_Z; the surface dissipation number, Di_{surf}; the heat production, H; the reference Rayleigh number, Ra; and the viscous dissipation, Φ. The thermal conductivity, k, is included in the heat diffusion term $\nabla \cdot (k\nabla T)$. Because conductivity is now considered to be heterogeneous, the diffusion of heat through hot (piles or plumes) and cold (downwellings) regions is reduced and enhanced, respectively.

Simulations are computed over a non-dimensional diffusion time of 0.0318, corresponding to 11.2 Gyr in dimensional units. Note that because they do not include mantle initial conditions, which are not known, and time-decreasing radioactive heating, our simulations are not meant to model the mantle evolution, and therefore durations should not be used to interpret specific sequences of events. The longer simulation time is necessary to allow the simulations to achieve a quasi-steady state, during which the surface and CMB heat flows oscillate around nearly constant values. Using this setup, we run 24 simulations exploring the impact of conductivity variations (Table 1) with values of n, K_D, and K_C in the range 0-0.8, 1-10, and 0.5-1.0, respectively. All observable and derived physical properties are averaged over a 2 Gyr window centred about $t = 4.5$ Gyr (illustrated in Figure 7) and are presented in Table 1. Complete details of the methods are included in the Supplement.

3 Results

To measure the evolution of the thermochemical structure, we examined our calculations once they became quasi-stationary, as defined by the mean core-mantle boundary heat flow, Q_{CMB}, and surface heat flow, Q_{SURF}. The stability of thermochemical reservoirs was assessed by their mean temperature, T_{prim}; average height, h_C (defined in the Supplement); and coverage of the CMB, A_{CMB} (Figure 3). The onset of instability, $t_{inst.}$, is calculated by examining time derivatives of average heights of primordial material (see the Supplement for details). We now examine the individual influence of conductivity changes with depth, temperature, and composition.

 ## 3.1 Effect of purely depth- dependent conductivity
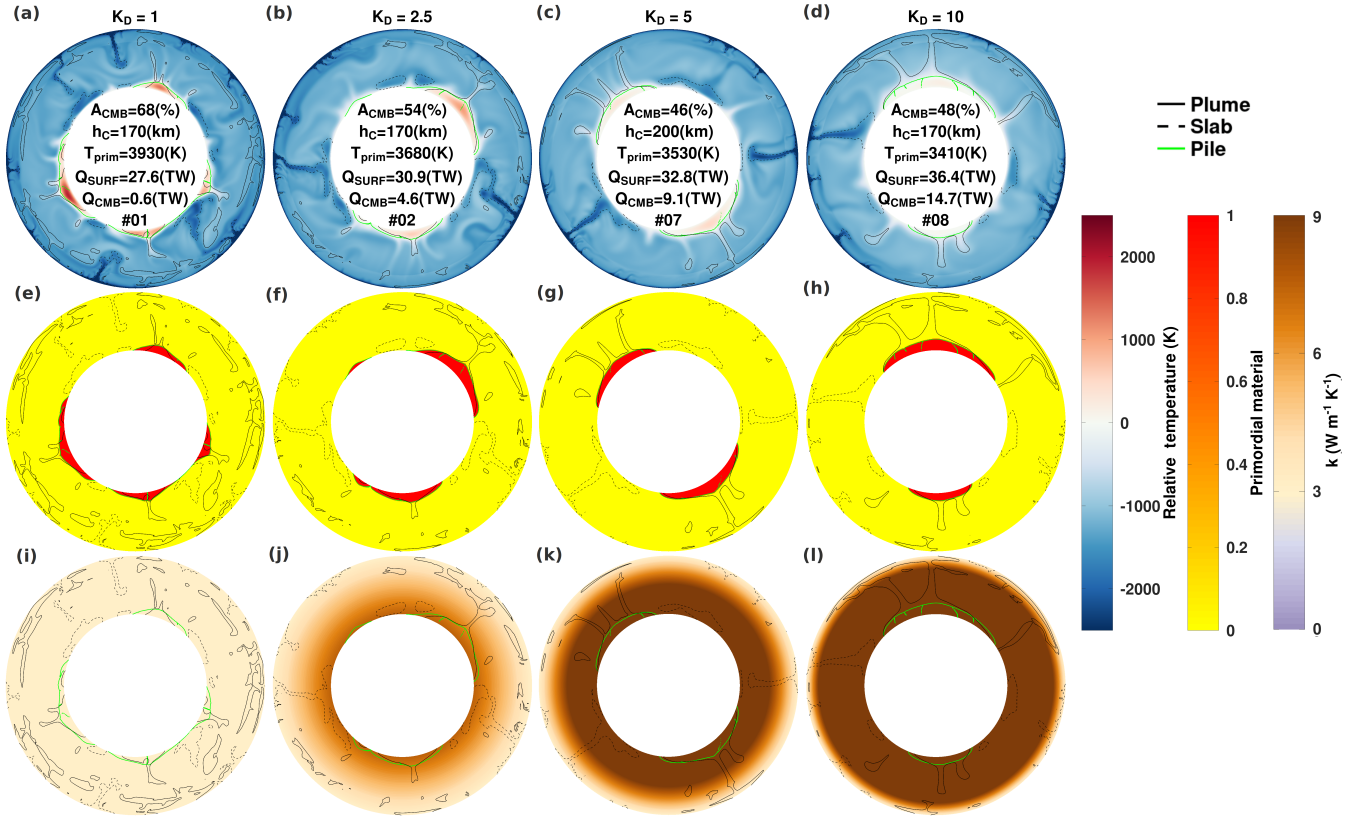
Figure 3. Temperature (relative to the CMB temperature) (top row), primordial material (centre row), and conductivity (bottom row) fields at 4.5 Gyr are shown as a function of K_D. Contours are indicated in the legend and field values are indicated on the colour bars. The conductivity colour bar saturates at 9 $\mathrm{Wm^{-1}K^{-1}}$ so that the values in (k) and (l) may be larger. Averaged properties and case numbers are inset.

First, we isolated the effect of purely depth- dependent conductivity. Relative temperature, primordial material, and conductivity fields are presented in Figure 3. The temperature fields are offset relative to the core-mantle boundary temperature to help illustrate temperature excesses (or deficits) within the piles. When K_D was increased from 1 to 10, we observed a decrease in the mean temperature of the piles (T_{prim}) (from 3930 K down to 3410 K), an increase in the mean mantle temperature (T_{mean}) (from 2150 K up to 2290).

From the primordial material fields, we observe that a modest conductivity gradient ($K_D = 2.5$) was sufficient to stabilize the thermochemical reservoirs and stimulates a 2-pile configuration (by 4.5 Gyrs) (compare plots (e) through (h)). This finding lends credence to pile configurations obtained by models that had adopted the canonical increase of conductivity by a factor of 2.5 from surface to core-mantle boundary. As K_D is further increased, reservoirs progress toward an antipodal arrangement. In

215   addition, the mantle flow becomes less turbulent since the increased thermal conductivity (and by extension thermal diffusivity) decreases the effective Rayleigh number.

The conductivity fields reflect a radially symmetric distribution with an increasing values from surface to CMB. This simplification is significant because heat flow between piles and ambient mantle and between the core and mantle is partially controlled by the lowermost mantle conductivities. Here, conductivity of the piles is identical to that of the laterally surround-

220   ing mantle. Comparing between each K_D case, for some arbitrary thermal gradient between piles and ambient mantle, a greater lowermost mantle conductivity will result in more efficient heat extraction; and thus a lower mean pile temperature. Furthermore, as lowermost mantle conductivity is increased, the heat flow at the core-mantle boundary is also increased (from 4.6 TW up to 14.7 TW, for K_D between 2.5 and 10). Note that the heat flows we observe encompass the lower and upper limits predicted for the Earth. The purely depth- dependent conductivity models we examined emulate the increase of thermal con-

225   ductivity with depth (and by extension, pressure). However, predicted thermal conductivities in the lowermost mantle do not greatly exceed 10 $\mathrm{Wm^{-1}K^{-1}}$. Therefore, temperature- dependence, which reduces the thermal conductivity, must be considered.

3.2   Effect of temperature- and depth- dependent conductivity

230   Next, we examine the added effect of temperature- dependence. Figure 4 shows the relative temperature and thermal conductivity fields for end-member cases featuring $K_D = 2.5$ and 10 (similar plot for $K_D = 5$ is shown in Supplement Figure S5), and Supplement Figures S3 and S4 plot the corresponding radial profiles. The effect of temperature clearly appears on the conductivity fields. Compared to the purely depth- dependent cases, thermal conductivity is strongly reduced throughout the mantle, and the depth dependence is strongly attenuated. By contrast, lateral variations in conductivity can be observed between

235   hot (less conductive) piles and cold (more conductive) downwellings. The lowest non-zero n value tested (i.e., 0.5) results in a 70% reduction in conductivity (from 7.5 $\mathrm{Wm^{-1}K^{-1}}$ down to approximately 2.2 $\mathrm{Wm^{-1}K^{-1}}$ (see conductivity profiles in Figure S3)) at the core-mantle boundary and a mean bottom-to-top conductivity ratio is < 1. This reduction is further amplified with greater n values. The piles evolving under these conductivity conditions move towards a more asymmetric configuration and may take on a columnar morphology (Figure 4(c)). Overall, temperature- dependence of conductivity results in a lower

240   conductivity at the bottom of the mantle, with mean bottom-to-top conductivity ratio < 1, which promotes thermochemical piles instability, as poorly conducting piles retain more heat and become more thermally buoyant. For $K_D = 10$, the thermal effect on conductivity as n was increased, could be compensated by the strong increase of conductivity with depth, and a mean bottom-to-top conductivity ratio larger than 1 was established (e.g., Figure 4 plots (k) and (l), resulting in a 2-pile arrangement). For instance, a mean conductivity ratio ≥ 2 is produced for $K_D = 10$ and $n = 0.5$. The horizontally averaged conductivities

245   near the CMB are brought closer to predicted values for the Earth's lower mantle (~ 8 $\mathrm{Wm^{-1}K^{-1}}$ (case #9)) and are much lower compared to the purely depth-dependent cases (30 $\mathrm{Wm^{-1}K^{-1}}$ (case #8), for $K_D = 10$; Figure S4). Interestingly, these cases result in a 2-pile arrangement thermochemical structure. Trade-offs between the temperature- and depth- effects on the lowermost mantle conductivity (and the mean bottom-to-top conductivity ratio) can be observed for cases featuring $K_D = 5$
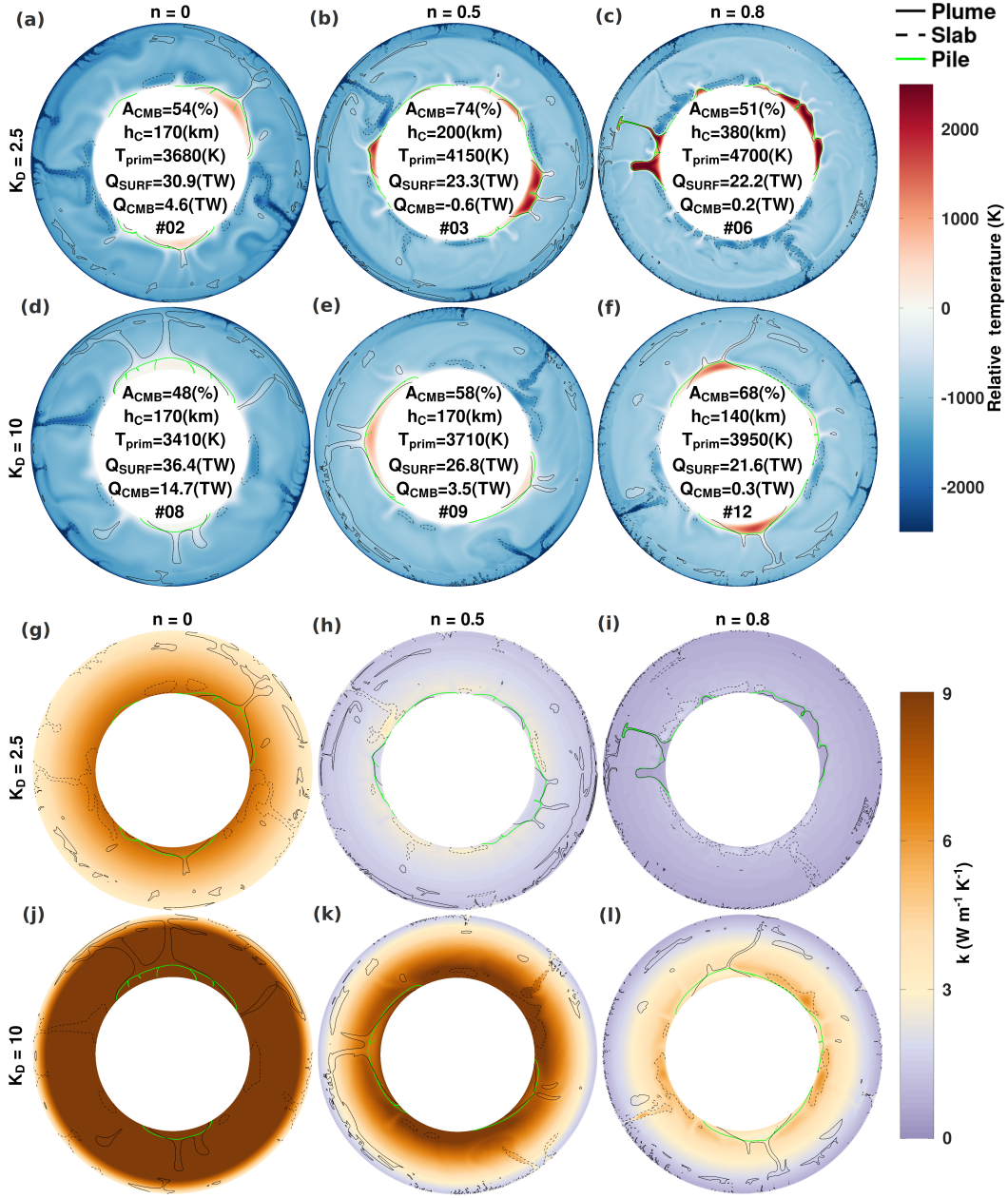
Figure 4. Temperature fields (relative to the CMB temperature) and conductivity fields at 4.5 Gyr are shown for cases as a function of K_D and n. Contours are indicated in the legend and field values are indicated on the colour bars. The conductivity colour bar saturates at 9 $Wm^{-1}K^{-1}$ so that the values in (j) and (k) may be larger. Averaged properties and case number are inset. (Primordial material fields are illustrated in Figure S2.)

(see Figure S5).

250   We observed that T_{prim} increased with greater temperature dependence (columns viewed left-to-right in Figure 4). In addition, temperature still decreased with an increased depth-dependent gradient, K_D (e.g., cases #4 and #10 and cases #5 and #11 in Figure 4), but in a lower extent than in the purely depth- dependent cases. Interestingly, for cases with a mean conductivity ratio < 1, T_{prim} is in excess of 500 K of the T_{CMB} (e.g., cases #1, #3 and #6 and cases S1, S2, and S4) resulting in locally negative bottom heat flux within piles. The evolution of the reservoirs in these cases tends to eventual entrainment. In those

255   systems, entrainment is typically preceded by columnar pile morphologies that become too thermally buoyant and eject blobs of thermochemical material. When piles retain much heat, temporal variations in the mean height of the piles due to thermal buoyancy are more rapid than the deformation by downwelling currents. The timing for the onset of instability, $t_{inst.}$, is listed for each case in Table 1. Pile's stability depends on how efficiently it can rid itself of heat. We find that greater heat extraction can be achieved for conductivity models characterized by $K_D = 10$ and that temperature dependence can emulate conductivi-

260   ties relevant to Earth's lowermost mantle. Because composition (i.e., iron enrichment) also attenuates piles' conductivity, this effect must be examined in conjunction with temperature and depth's influence on the mantle's mean conductivity ratio.

Table 1. Averaged properties for all cases presented. Supplemental cases are indicated by a letter 'S'. All values are computed within in a 2 Gyr period encompassing 4.5 Gyr.

Case #	K_D	K_C	n	T_{mean} (K)	T_{prim} (K)	global rms dT_{prim} (K)	negative rms dT_{prim} (K)	positive rms dT_{prim} (K)	$\Delta T_{prim,max}$ (K)	Q_{SURF} (TW)	Q_{CMB} (TW)	h_C (km)	$A_{CMB}(\%)$	$t_{inst.}$ (Gyr)
1	1	1	0	2150	3930	450	350	550	1400	27.6	0.6	170	68	5.8
2	2.5	1	0	2200	3680	280	220	330	770	30.9	4.6	170	54	9.2
3	2.5	1	0.5	2370	4150	610	510	720	1480	23.3	-0.6	200	74	5.2
4	2.5	0.8	0.5	2380	4330	670	600	740	1530	24.1	1.1	290	55	4.9
5	2.5	0.5	0.5	2390	4420	740	660	830	1830	23.3	0.5	400	64	4.5
6	2.5	1	0.8	2500	4700	770	750	790	1620	22.2	0.2	380	51	4.5
7	5	1	0	2230	3530	150	130	170	400	32.8	9.1	200	46	>11.2
8	10	1	0	2290	3410	90	110	80	190	36.4	14.7	170	48	>11.2
9	10	1	0.5	2400	3710	260	210	320	730	26.8	3.5	170	58	>11.2
10	10	0.8	0.5	2410	3850	360	300	440	870	26.3	4.6	200	46	8.4
11	10	0.5	0.5	2390	3760	320	270	370	890	24.8	3.5	170	58	9.0
12	10	1	0.8	2490	3950	470	380	570	1200	21.6	0.3	140	68	8.2
13	DH	1	0	2260	3400	90	120	70	710	37.6	13.5	170	53	>11.2
14	DH	0.8	0	2250	3450	110	120	110	270	38.5	15.5	200	41	>11.2
15	DH	1	0.5	2370	3620	200	170	230	560	26.6	3.3	140	60	>11.2
16	DH	0.8	0.5	2380	3700	270	220	330	780	26.5	3.6	170	59	11.1
17	DH	0.5	0.5	2380	3820	420	320	520	1110	25.6	3.0	170	64	8.8
18	DH	0.8	0.8	2470	4190	530	480	580	1170	22.7	1.5	200	49	6.6
S1	1	1	0.5	2380	4640	770	780	770	1540	23.7	1.0	750	36	3.9
S2	1	1	0.8	2510	4900	820	830	810	1780	21.8	0.6	930	36	4.1
S3	5	1	0.5	2400	4050	490	400	580	1230	25.2	2.3	200	47	6.0
S4	5	1	0.8	2490	4380	680	640	710	1430	21.4	0.0	200	61	5.4
S5	5	0.8	0.5	2400	4160	560	480	640	1330	24.5	2.4	200	47	5.6
S6	5	0.5	0.5	2410	4210	620	530	730	1530	23.9	1.7	230	57	5.2

3.3 Including the effect of composition- dependent conductivity
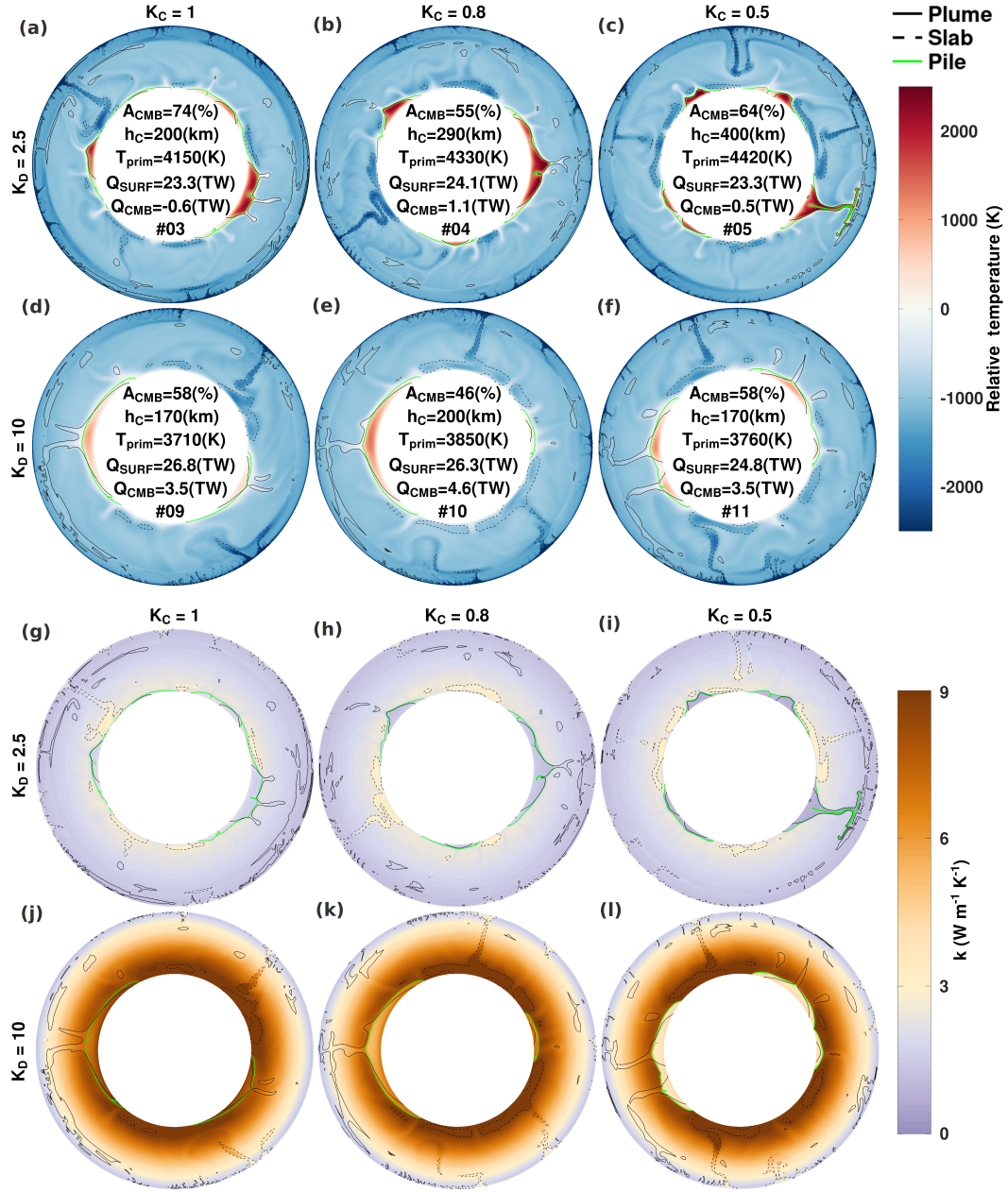
Figure 5. Temperature (relative to the CMB temperature) and conductivity fields at 4.5 Gyr are shown as a function of K_D and K_C when $n = 0.5$. K_C is increases from right to left. Contours and inset values are defined similarly as in Figure 4. The conductivity colour bar saturates at $9\,\mathrm{W\,m^{-1}K^{-1}}$ so that the values in (j), (k), and (l) may be larger. (Primordial material fields are illustrated in Figure S6.)

The effect of compositional correction is highlighted in Figure 5 for the cases featuring $K_D = 2.5$ and 10 with $n = 0.5$. For the cases featuring $K_D = 2.5$, composition- dependence further reduces the conductivity of piles below the conductivity of the ambient mantle at lowermost mantle depths (Figure 5 panels (h) and (i)). Although small, the reduction of pile conductivity due to composition- dependence amplifies the behaviour observed for temperature- dependent cases with similar depth- dependence (i.e., a decrease in the piles' stability) and results in earlier instability (see Figure S11).

Similarly, for the $K_D = 10$ case, accounting for compositional dependence of conductivity amplifies the effects induced by temperature- dependence. In addition, the magnitude of the reduction in conductivity is also amplified. The percentage conductivity difference at a depth of 2500 km (i.e., at a depth adjacent to the bulk of the piles) is approximately 40% when $K_C = 0.8$ approximately 60% and when $K_C = 0.5$. This conductivity difference between piles and the ambient mantle induces a minor increase in pile temperature that grows over time. When $K_C = 0.8$, this increase in temperature leads to a slowly manifesting thermal instability that results in a bulk ejection of thermochemical material by 8.4 Gyr. However, the entrainment of the piles does not occur shortly after this episode of ejection (see Figure S12).

For the intermediate depth- dependent case $K_D = 5$ (Figure S9), the mean lowermost mantle conductivity is greater than the surface conductivity and does not vary significantly when the conductivity of primordial material is reduced (i.e., < 1 $\mathrm{Wm^{-1}K^{-1}}$ in the lowermost mantle; Figure S10). The maximum conductivity, characterized by the remnant downwelling material localized within the bottom 300 km, is approximately 2 $\mathrm{Wm^{-1}K^{-1}}$ higher than the mean conductivity profile. The minimum conductivity, characterized by the hottest regions of the reservoirs, is approximately 2 $\mathrm{Wm^{-1}K^{-1}}$ lower than the mean, and is localized near the tops of the piles, where the hottest and most buoyant primordial material accumulates (approximately 500 – 800 km above the CMB). Pile temperature marginally increased when K_C was reduced. The additional thermal buoyancy imparted into the piles quickened the onset of instability. For this K_D value, the erosion of piles is initiated approximately 0.4 Gyr and 0.8 Gyr earlier from 6 Gyr when $K_C = 0.8$ and $K_C = 0.5$, respectively. Furthermore, pile configuration may change. When $K_C < 1$, single pile configuration can be attained as early as 8 Gyr (Figure S13). At all depth- dependences tested, we found that the effect of composition- dependence was small compared the dominant temperature- dependent effect. Nevertheless, as depth- dependence was greatly increased, the compounded conductivity reduction became greater, and introduced a slowly manifested thermal instability. Thus, a much earlier bulk ejection of thermochemical material was observed compared to cases where the composition effect was absent.

3.4 Long-term stability of thermochemical reservoirs featuring mineral physics derived conductivities
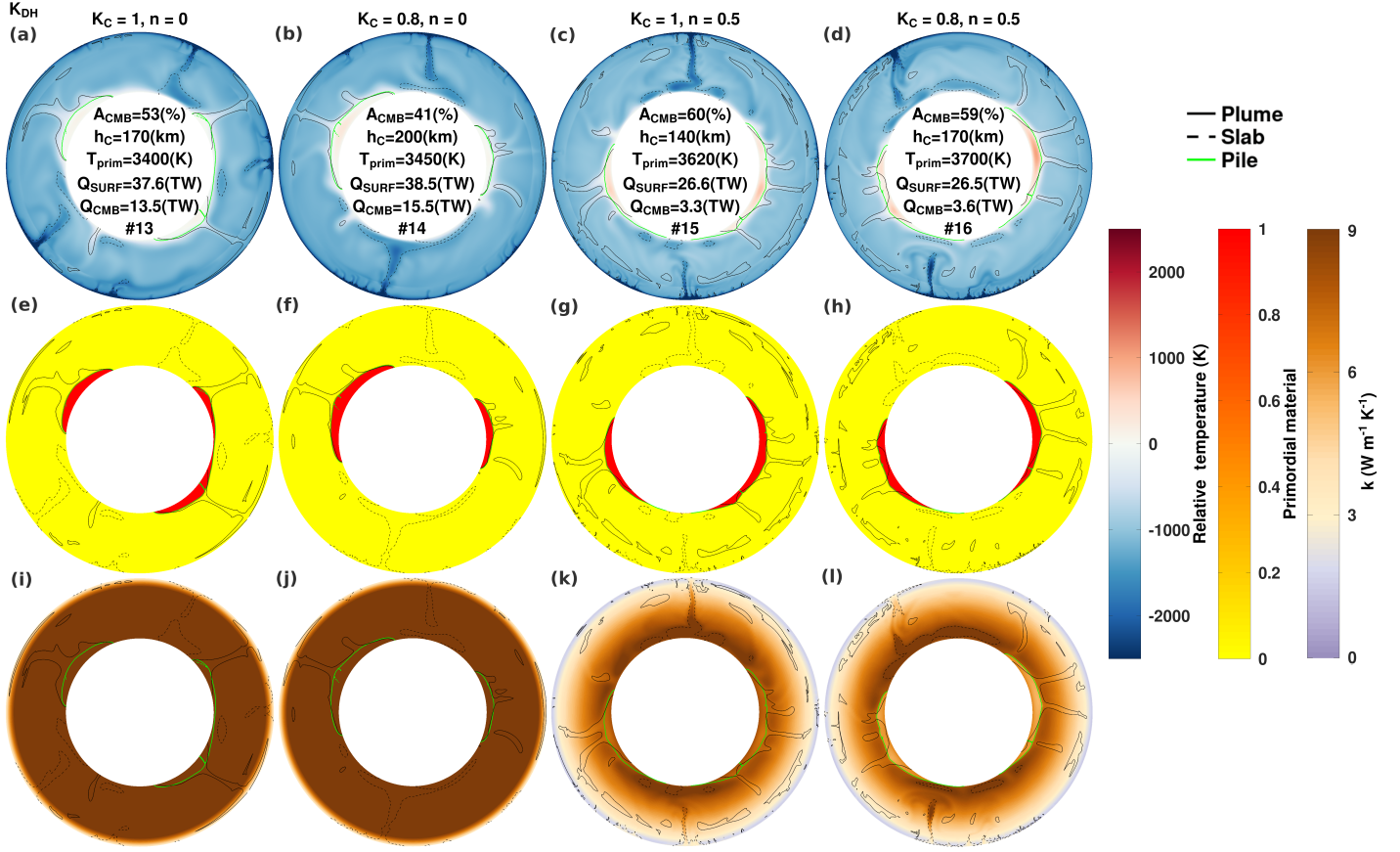
Figure 6. Temperature (relative to the CMB temperature) (top row), primordial material (middle row), and conductivity (bottom row) fields at 4.5 Gyr are shown for cases featuring K_{DH}. Contours and inset values are defined similarly as in Figure 4. The conductivity colour bar saturates at 9 $\mathrm{Wm^{-1}K^{-1}}$ so that the values in (i) - (l) may be larger. Inset values are defined similarly as in Figure 4.

Finally, we examine the effect of depth- dependence, based on measured conductivities of upper and lower mantle minerals (Hsieh et al., 2017, 2018), on the long-term stability of thermochemical reservoirs. First, we isolate the effects of temperature- ($n = 0.5$) and composition- ($K_C = 0.8$) in conjunction with mineral conductivities. Second, we construct the fully heteroge-
neous thermal conductivity model ($n = 0.5$ and $K_C = 0.8$ case #16), which we use as a reference case. We find that the resulting lower mantle conductivities for this reference case are comparable to current estimates (e.g., Geballe et al., 2020). Figure 6 indicates that for given values of n and K_C, models obtained with the mineral physics depth- dependence are very similar to those obtained with linear depth dependence with $K_D = 10$ (see Figure 4 and 5 for comparison). Heat flows for our models reached a quasi-steady state by approximately 4 Gyr (Figure 7). We found that temperature- dependent conductivity greatly reduced both CMB and surface heat flows (by approximately 73% and 30%, respectively), as less heat can be extracted from
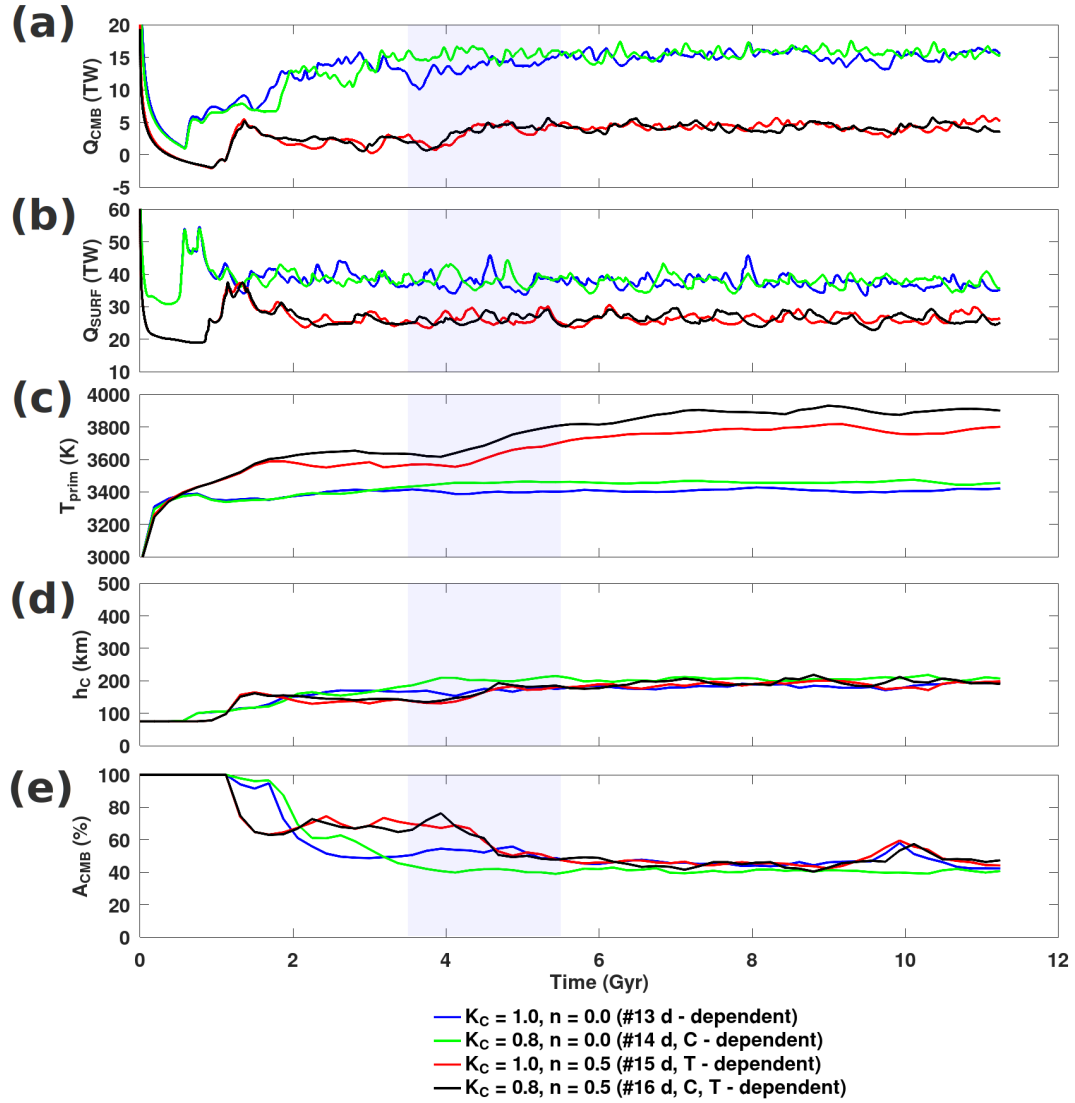
Figure 7. Evolution of cases featuring K_{DH} corresponding to those presented in Figure 6. The quasi-stationary period centred about 4.5 Gyr is shaded in gray.

the base. Furthermore, we find that composition- dependence is of secondary importance, in agreement with Li et al. (2022)'s findings. Despite a 20% reduction in the conductivity of primordial material (green), Q_{CMB} is marginally greater (by 2 TW). Similarly, Q_{CMB} is marginally greater when temperature- dependent conductivity included composition- dependence (by 0.3 TW). This behaviour is likely owing to less CMB coverage in composition- dependent cases. Differing conductivity conditions can result in many thermochemical reservoir evolution and cooling histories. For the cases examined in Figure 6, we found that the mean height of piles and CMB coverage approached a quasi-steady value. However, T_{prim} greatly increased when

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temperature dependence was considered. For systems with a temperature- dependent conductivity (i.e., red or black curves), piles slowly heat up during their long-standing CMB coverage. Piles' gained thermal buoyancy increased their height (thus, liberating the core-mantle boundary surface) and allowed more heat to be extracted from the core. Determining the mechanisms that trigger different outcomes will provide constraints for plausible mantle conductivity models.

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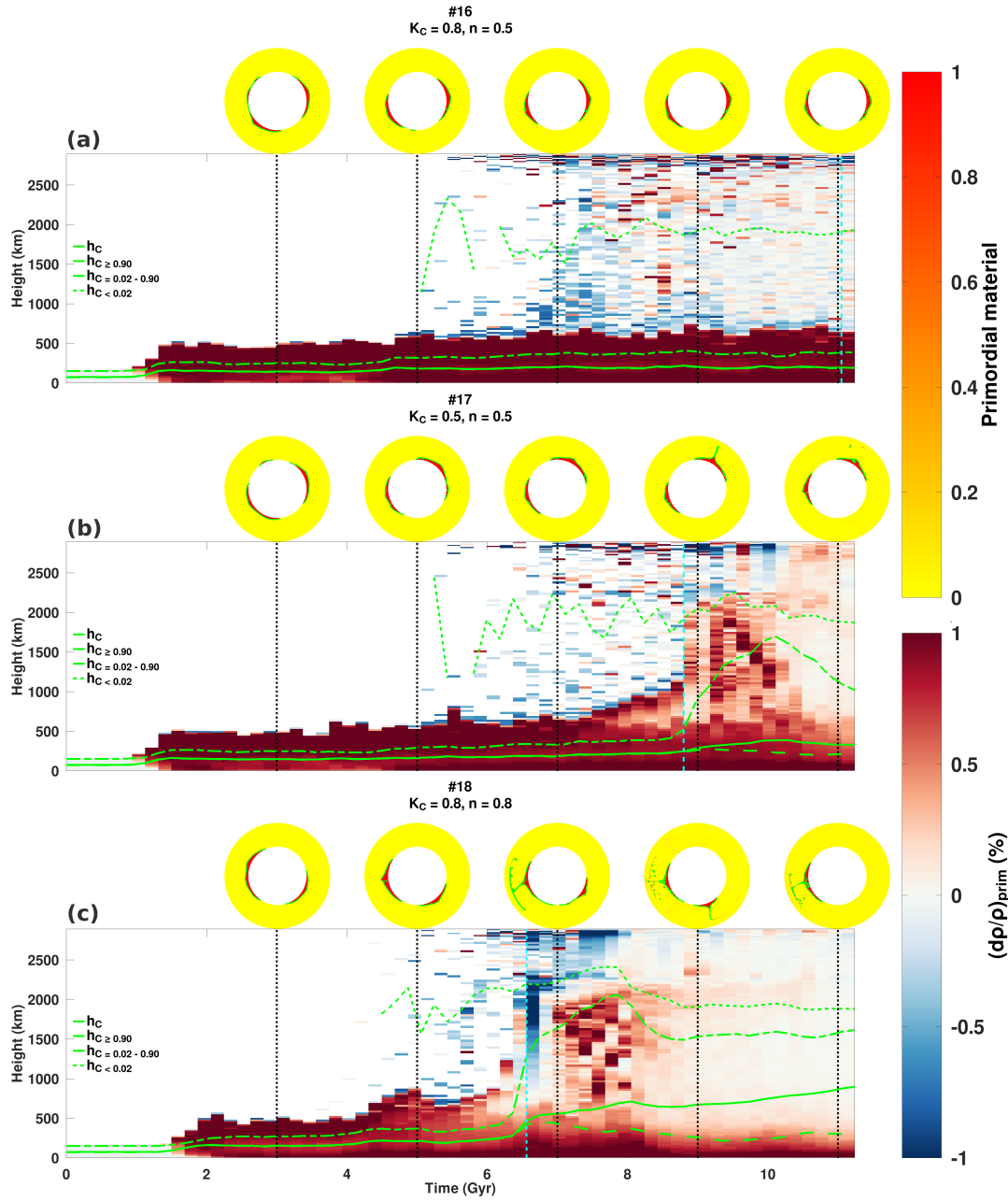
Figure 8. Evolution of the horizontally averaged primordial material density anomalies is illustrated for cases featuring K_{DH}. Primordial field snapshots are sampled at 2 Gyr intervals starting at 3 Gyr above the timeseries (dashed-black vertical line indicates the time). Mean heights of primordial material are plotted on top of the density anomaly timeseries. The dashed-cyan vertical line indicates the onset of instability in thermochemical reservoirs. Piles are indicated similarly as in Figure 3.

Figure 8, plotting the heights of primordial material (for different ranges of composition concentration) in conjunction with the horizontally averaged density anomalies as a function of time, illustrate the evolution of the thermochemical structure for cases with different n and K_C. Because the horizontally averaged profiles mask the spatial distribution, primordial field snapshots with 2 Gyr intervals are also indicated for reference. Figure 8 may be used to examine departures from reference moderate temperature- dependence ($n = 0.5$) and compositional- dependence ($K_C = 0.8$) (case #16). The variations in average height do not discriminate between 'intrinsic' (i.e., thermal buoyancy) or 'extrinsic' (i.e., downwellings) deformation. However, the influence of downwellings can be observed following the transient period. The first downwellings impinge on the initial dense layer but do not result in a rapid uplift of material (sufficient to eject blobs of dense material). Once the initial dense layer has organized into piles, downwellings tend to move dense material laterally over the CMB but not rapidly increasing the pile height. Nevertheless, we find that it is easier for downwelling currents to push primordial material that has been made lighter due to their retained heat.

In the reference case, thermochemical convection exhibits a stable 2-pile configuration during the entire simulation. The total pile height can be roughly read from the density anomaly plot (i.e., the initial sharp contrast in colour between red and white). For stable piles, the average heights of the pile (h_C) will then be roughly less than half of their total height. (Average height is calculated based on volumetric weighting in a spherical geometry (see Supplement Section 3.3).) These primordial reservoirs remain highly concentrated with a thin veneer of less concentrated material (from chemical diffusion with the ambient mantle) covering the piles. Thus, the average height of the veneer ($h_{C=0.02-0.90}$) is slightly greater than the average height of the piles because it is localized at the top and sides of the reservoirs. This is a good quantity to analyse for temporal variations, since this veneer surrounds buoyant thermochemical material structures (i.e., columnar plumes or ejected blobs). For this conductivity model, the slow erosion of the least concentrated primordial material ($C < 0.02$) from this veneer occurs after 5 Gyr. From the temporal variations in average heights, we find that thermal instability appears to manifest very late in the simulation run time (after approximately 11 Gyr).

When only K_C is reduced, from 0.8 to 0.5 (#17), a 2-pile configuration is also maintained throughout the simulation, but episodes of bulk erosion in thin plume conduits are possible (e.g., around 9 Gyr). Following the erosion of light material, the long-term build up of heat in the thermochemical pile (from 7 to 9 Gyr) manifests a less dense region localized towards the top of the pile. By 9 Gyr, the density anomaly plot is dominated by an upwelling that extends to the base of the upper mantle. Following the impingement of the plume (from 9 to 11 Gyr), a fallout of dense blobs of primordial material are circulated about the mid-lower mantle. Compared with cases with lesser depth- dependence, the effect of composition dependence appears to have a greater influence on thermal instability (see cases #4 and #5 in Figure S11 compared with cases #16 and #17 in Figure 8). A lesser depth- dependence implicitly makes temperature- dependence the dominant factor in heat exchange. Thus, the effect of composition will easily be overshadowed.

When only n is increased from 0.5 to 0.8 (#18), the onset of instability occurs approximately 5 Gyr sooner. Because it is more temperature dependent, thermal conductivity is reduced, which makes the heat transfer between the piles and the ambient mantle poorer. From 5 to 7 Gyr, similarly with case #17, the piles' retention of heat results in a reduced density anomaly (relative to the bulk pile). The ejection of primordial material from the largest of the two reservoirs occurs at 6.6 Gyr. The

fallout blobs of thermochemical material are circulated in the lower mantle but are mainly localized above the pile. After 9 Gyr, the smaller pile is pushed by downwelling currents, and by 11 Gyr the piles coalesce.
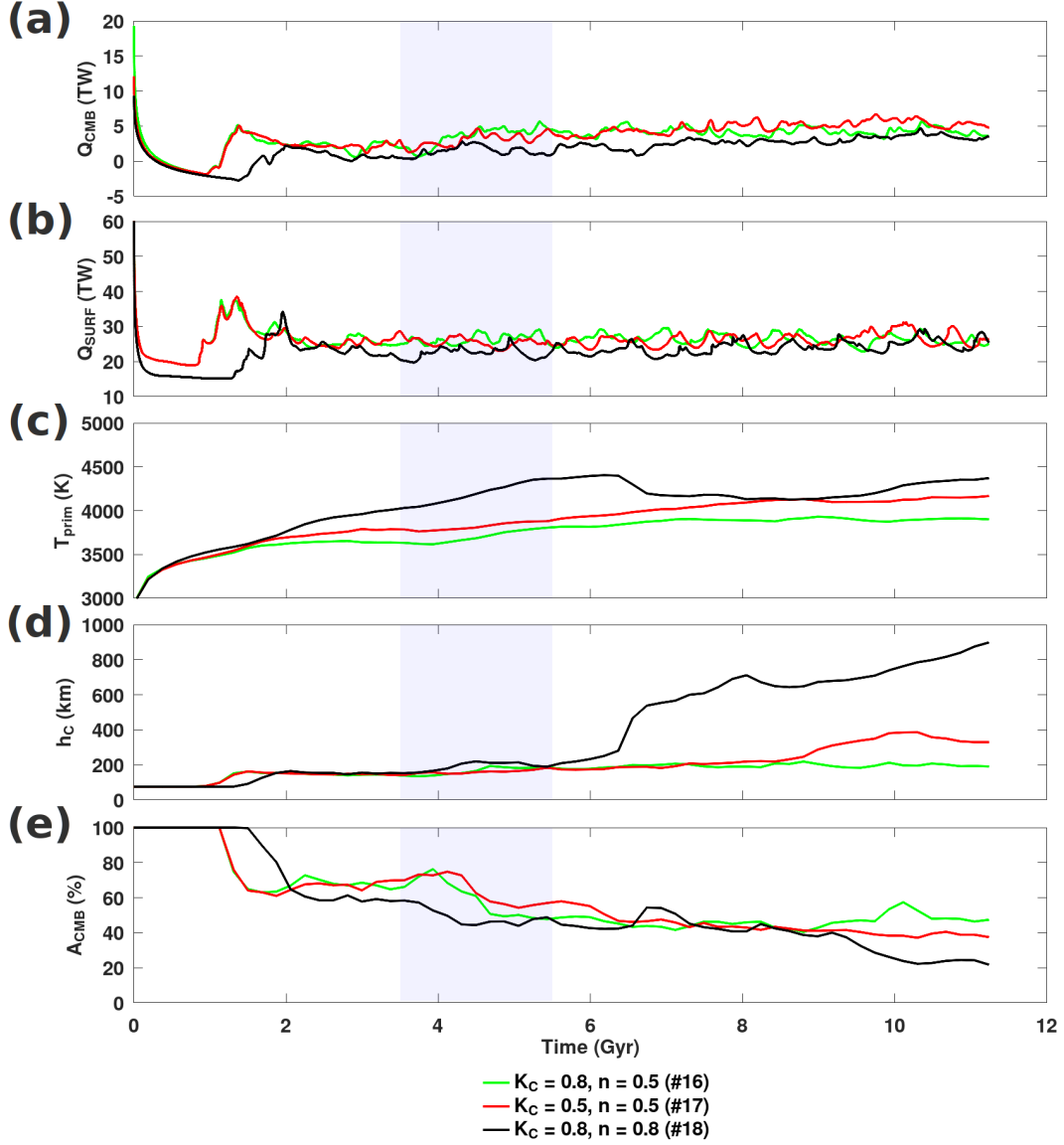
Figure 9. Evolution of cases corresponding to Figure 8. The quasi-stationary period centred about 4.5 Gyr is shaded in gray.

350   Examining the timeseries for the cases presented, T_{prim} increased marginally due to compositional correction and increased significantly with temperature dependence (see Figure 9). In general, T_{prim} increases when thermochemical reservoir conductivity is reduced i.e., temperature- dependence (and, to a lesser extent, composition dependence) is strong. Only until h_C had

increased (indicating that piles became unstable and started eroding) T_{prim} decreases (i.e., case #18). Temperature- dependence greatly amplifies T_{prim} and is the dominant effect over composition. The long-term evolution of reservoirs characterized

355 by a marginal temperature increase may result in a stable arrangement of piles with increased topography with respect to the initial layering (see Figure 6, #16), whereas, a substantial increase in temperature (i.e., exceeding approximately 500 K) may lead to the entrainment of piles (see Figure 8, #18). Between these two cases, the onset of instability differs by approximately 4.5 Gyr. The differences in system's conductivity fields (profiles and bottom-to-top conductivity ratios) clarify these observations.

360 The distribution of light material ($C < 0.02$) is scattered about the lower mantle and may be ejected in small amounts into the upper mantle. An initial negative density anomaly is established compared with the mean mantle density (which is dominated by cold downwelling structures). When the thermochemical reservoirs finally become unstable, material with C between 0.02 and 0.90 is rapidly lifted away from the piles. This material dominates the mean density profile and produces a positive anomaly. The onset of light erosion precedes the onset of instability and the period between light and heavy erosion is reduced

365 when the mean conductivity gradient is reduced (e.g., dotted and dot-dashed curves in Figure 8, and Figure S14. Interestingly, the radial conductivity profile obtained by models #16 and #17 lead to average CMB conductivity (and lower mantle conductivities) within values estimated from mineral physics (i.e., between 3 and 10 $\mathrm{Wm}^{-1}\mathrm{K}^{-1}$) (Hsieh et al., 2018; Deschamps & Hsieh, 2019; Geballe et al., 2020) (see Figure S14). However, the mean conductivity values in the lower mantle obtained by #18 span the lower end of current estimates.

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4   Discussion

The evolution of thermochemical reservoirs depends on their temperature and on the mean bottom conductivity. The value of bottom conductivity results mainly from the competing thermal and pressure effects. That is, stronger temperature- dependence (larger n) reduces conductivity, which may or may not compensate (or be exceeded by) depth- dependence (larger K_D). Considering the purely depth- dependent conductivity scenario, heat flow between reservoirs and the surrounding mantle may attain a rate that inhibits reservoir temperature increases due to enrichment in HPEs. That is, a greater lower mantle conductivity stabilizes thermochemical reservoirs by mitigating any (additional) thermal buoyancy imparted by internal heat sources and by increasing heat diffusion in regions where hot instabilities grow. When temperature- dependence (and, to a lesser extent, composition- dependence) is considered, the conductivity of reservoirs is reduced with respect to the surrounding mantle. If the depth- conductivity ratio is insufficient to compensate for this conductivity reduction, a negative feedback loop forms whereby a poorly conducting pile cannot evacuate heat, becomes hotter, and further reduces its conductivity. The imparted thermal buoyancy destabilizes the reservoirs and influences CMB coverage configuration, erosion rate, and the onset of entrainment.

The effect of composition- dependence on the stability of thermochemical reservoirs is secondary to the thermal effect. For conductivity models with near-unity bottom-to-top conductivity ratio (when thermal and depth- dependent effects nearly compensate each other, greater compositional correction may quicken the onset of instability (e.g., by less than 1 Gyr, comparing cases S#5 and S#6; Figure S13). When depth- dependence is greater, a greater bottom-to-top conductivity ratio is implied which acts to stabilize the piles. However, the amplitude of conductivity variations is also increased. Thus, a greater composition-dependence may quicken the onset of instability (e.g., by approximately 2 Gyr, comparing cases #16 and #17; Figure 8) but take a longer period of time to manifest (e.g., by approximately 4 Gyr, comparing cases S#6 and #17).

Variations in the physical properties of thermochemical reservoirs, most notably the buoyancy ratio and enrichment in HPEs, have an influence on their long-term evolution. Constraints on these properties are still being determined and subjects of ongoing research. Given the scope of this study, isolating the effect of conductivity on stability may be masked by their first order influences. For example, greater composition- dependence for conductivity is related to pile's enrichment in iron and thus implies density increase requiring an increase in buoyancy ratio. In contrast, amount of enrichment in HPEs will directly influence the thermal buoyancy and destabilize piles in the long-term. Furthermore, we do not consider a decaying rate of internal heating. Assuming a mean 3 Gyr half life, internal heating rate should be reduced by almost an order of magnitude by the end of the simulation period we consider. It may be possible that the stronger influence of thermal buoyancy is limited to earlier periods of maximum heat input. The influence of these parameters in conjunction with the moderate heterogeneous conductivity profile we propose (i.e., case #16) should be examined in further detail.

The core-mantle boundary temperature may also be an important factor in the stability and evolution of thermochemical reservoirs when a heterogeneous conductivity is considered. In our study, the reference state imposes a CMB temperature ($T_{CMB} = 3440$ K) that is on the lower end of the estimates (e.g., Lay et al., 2008; Mosca et al., 2012; Nomura et al., 2014). Boehler (2000); Price et al. (2004) and Kawai & Tsuchiya (2009) suggest greater temperatures, in excess of 3750 K and up to 4000 K, are possible. For the constant system heating conditions we consider, a greater CMB temperature implies that the

mean temperatures in the lowermost mantle will also be increased, resulting in a lower thermal conductivity in that region and within the piles. In addition, higher thermal gradients at the base of the mantle will result in an increase in mean CMB heat flow. Thus, at very high CMB temperatures piles may become unstable. However, stable piles (under hotter conditions) can be accommodated by considering a lower n or a greater depth- dependent conductivity, or by other physical parameters (e.g., temperature- dependence of viscosity, or buoyancy ratio). Therefore, conclusions drawn from our results should be unchanged. Because a cooling bottom boundary is not considered, it is possible that piles evolving with our CMB temperature (or in hotter systems) could become more stable as the mantle cools and the mean lowermost mantle conductivity (and potentially the CMB heat flow) rises. However, examining evolving system heating conditions is out of the scope of our study.

Alternative formulations of the lattice conductivity exist in the literature featuring temperature and density dependences (e.g., Manthilake et al., 2011; Okuda et al., 2017). Furthermore, measurements of the temperature dependent exponent for lower mantle materials may take on values that are less than 0.5 (i.e., between 0.2 and 0.47). For the lattice conductivity we consider, a lower exponent (lesser temperature dependence) will promote stability in piles. In addition, the radiative component of conductivity is much less than the lattice component for temperatures less than the CMB temperature (e.g., Dubuffet et al., 1999). It may be possible that the piles' temperature increases we observe could curb the conductivity reduction due to the lattice component. We do not rule out these possibilities but propose that different conductivity formulations are subjects for future studies.

5   Conclusions

In this study, we investigate the influence of variations in thermal conductivity on thermochemical convection, and find that a heterogeneous conductivity strongly influences the long-term evolution of thermochemical reservoirs. The combined influences of temperature- and depth- variations determines the mean conductivity ratio from bottom-to-top. In the calculations we present, for the mean conductivity profile to be comparable to the conductivity often assumed in numerical models, the depth-dependent ratio must be at least 9 times the surface conductivity. The composition- dependence for conductivity only plays a minor role that augments and behaves similarly to a small conductivity reduction due to temperature. Nevertheless, this effect may be amplified when depth- dependence is increased. For the cases we examine, when the mean conductivity in the lowermost mantle is much greater than the surface conductivity, large reservoirs can be maintained until the end of the simulation.

Code and data availability. The numerical code is available by reasonable request to Paul James Tackley. The data corresponding to the numerical simulations are too large to be stored online, but they can be requested from the corresponding authors as well as the input files used to run the simulations.

Author contributions. Joshua M. Guerrero: contributed to the study design, formal analysis, visualization, and writing - original draft preparation. Frédéric Deschamps: contributed to the study design, investigation, visualization, writing - review & editing. Yang Li: contributed to writing - review & editing. Wen-Pin Hsieh: contributed to consultation on the thermal conductivity model and writing - review & editing. Paul J. Tackley: contributed to software by designing the 3D thermochemical convection code and writing - review & editing. All authors collaborated and contributed intellectually to this paper.

Competing interests. The authors declare that they have no conflict of interest.

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