

The conductive cooling of planetesimals with temperature-dependent properties

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Key Points:

- Conductivity, heat capacity and density are temperature dependent and control the cooling of planetesimals
- Conductive cooling models of meteorite parent bodies frequently approximate these properties as constant
- Temperature-dependence in a model of the pallasite parent body delays the onset of core solidification by 40 million years

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Abstract

Modelling the planetary heat transport of small bodies in the early Solar System allows us to understand the geologic context of meteorite samples. Conductive cooling in planetesimals is controlled by thermal conductivity and volumetric heat capacity, which are functions of temperature (T). We investigate if the incorporation of the T -dependence of thermal properties and the introduction of a non-linear term to the heat equation could result in different interpretations of the origin of different classes of meteorites. We have developed a finite difference code to perform numerical models of a conductively cooling planetesimal with T -dependent properties and find that including T -dependence produces considerable differences in thermal history, and in turn the estimated timing and depth of meteorite genesis. We interrogate the effects of varying the input parameters to this model and explore the non-linear T -dependence of conductivity with simple linear functions before applying non-monotonic functions for conductivity and volumetric heat capacity fitted to published experimental data. For a representative calculation of a 250 km radius pallasite parent body, T -dependent properties delay the onset of core crystallisation and dynamo activity by ~ 40 Myr, approximately equivalent to increasing the planetary radius by 10%, and extends core crystallisation by ~ 3 Myr. This affects the range of planetesimal radii and core sizes for the pallasite parent body that are compatible with paleomagnetic evidence. This approach can also be used to model the T -evolution of other differentiated minor planets and primitive meteorite parent bodies and constrain the formation of associated meteorite samples.

Plain Language Summary

Meteorites are fragments of the earliest planetary building blocks in our Solar System. These small planetary bodies (planetesimals) were a few tens to hundreds of km across. Different types of meteorites came from different planetesimals of various sizes. Some types of meteorites formed near the surface of their parent bodies, while others are derived from deep within the planetesimal, where it stayed hotter for longer. Understanding how quickly these planetesimals cooled allows us to match the cooling rates recorded within meteorites to different depths inside their parent body: the rock that formed the meteorite would have cooled rapidly near the surface and more slowly nearer the centre.

Properties such as thermal conductivity, heat capacity and density control how quickly planetesimals cool down. These properties are temperature dependent, meaning their value changes as the temperature of the material changes. If we understand these properties, we can better model how quickly planetesimals cooled in the early solar system. Previous models have often approximated these effects with constant values. In this work we use properties that change as the temperature of the planetesimal changes, and investigate how much of an impact this makes on the cooling history.

We find that temperature dependent properties produce different results to constant values, which can lead to different estimations of the size of the parent body for certain meteorites, whether some groups of meteorites formed in the same body, and when the core of these parent bodies may have frozen solid.

1 Introduction

Planetesimals are small rocky or icy bodies of a few to a few hundred kilometres in diameter that formed through coagulation of dust grains in the protoplanetary disk, and are considered the building blocks of larger planetary bodies (Kokubo & Ida, 2012). These early planetesimals are hypothesised to be the primary parent bodies of meteorites while the remnants of disrupted planetesimals, preserved as asteroids, are termed the secondary parent bodies (Greenwood et al., 2020). Planetesimals experienced varied ther-

mal histories: differentiated meteorites displaying igneous textures are sourced from planetesimals that underwent melting and segregation of a metallic core and silicate mantle (Baker et al., 2005), while chondritic meteorites contain primitive material including solids that condensed from hot gas in the Solar Nebula (MacPherson, 2014). Understanding the geological context of differentiated meteorites and their parent bodies' thermal evolution allows constraints to be placed on the formation, differentiation and eventual breakup of planetesimals, and on the early evolution of the Solar System. In this context, models of conductive cooling of differentiated primary parent bodies are frequently used to aid the interpretation of meteorite samples. In this study we investigate the importance of including temperature dependent thermal properties in such models. We use a pallasite parent body as an example to illustrate the influence including T -dependent properties can have on understanding the origin of meteorite samples.

One approach to understanding the formation of meteorites is to analyse the thermal processing experienced by meteorite samples and to compare this to estimated temperature conditions within the parent body using thermal evolution models. Heat flow in conductively cooling planetesimals is controlled by the material properties of their constituent minerals — thermal conductivity (k), density (ρ) and heat capacity (C), in addition to the boundary conditions imposed and the geometry of the planetesimal. Large temperature gradients are expected in planetesimals, with typical surface temperatures of ~ 250 K rising to ~ 1800 K at the centre (Bryson et al., 2015; Scheinberg et al., 2015). Planetesimals are low pressure environments, with a gradient of ~ 0.3 GPa calculated across a 250 km radius silicate body with a 125 km radius iron core (see hydrostatic equilibrium calculation in supplementary information). If k , ρ and C are assumed constant, they can be expressed in terms of diffusivity $\kappa = \frac{k}{\rho C}$. This is a common approximation made in conductive cooling models of differentiated planetesimals despite temperature and pressure dependence (Bryson et al., 2015; Fu et al., 2014; Haack et al., 1990; Tarduno et al., 2012). While the finite difference methods frequently used in these models can be applied to systems involving T -dependent properties, the heat conduction equation becomes nonlinear and more expensive to solve when T -dependent k is included (Özışık, 1993). Conductivity decreases by 40 – 60 % of its original value in metamorphic and igneous rocks when temperature increases from room temperature to 1273 K, while conductivity increases by approximately 4 % with an increase in pressure of 1 GPa (Hofmeister, 1999; Seipold, 1998; Wen et al., 2015). Due to the weaker dependence of conductivity on pressure, and the low pressure gradients expected in planetesimals, in this paper we will focus on the temperature dependence of material properties.

In solids at low temperatures ($T < \theta_D$, the Debye temperature), heat capacity increases from zero at 0 K as $C_v \sim AT^3$, where C_v is specific heat capacity at a constant volume and A is a constant (Debye, 1912). At high temperatures ($T > \theta_D$), heat capacity is weakly dependent on temperature and can be approximated with a constant value (Petit & Dulong, 1819). This results in approximately 30 % increase in C over the temperature range commonly modelled for planetesimals (Figure 1).

In electrically insulating solids such as mantle silicates, heat is primarily transferred through lattice or phonon conduction. As temperature increases, the mean energy per phonon also increases due to the change in phonon specific heat. At lower temperatures ($T < \theta_D$), the inelastic phonon relaxation time is constant as scattering is primarily due to crystal defects or boundaries. This results in $k \propto T^3$ due to the T -dependence of C (Hofmeister, 1999; Poirier, 2000). When phonon momentum exceeds a threshold at high temperatures, phonon–phonon Umklapp scattering acts to reduce k , producing a $k \propto \frac{1}{T}$ dependency (Poirier, 2000). This non-monotonic behaviour is illustrated in Figure 1.

A change in density with temperature can be linked to thermal expansion by the coefficient of expansivity, α : $\rho = \rho_0 - \alpha\rho_0(T - T_0)$, where ρ_0 is a reference density at T_0 , commonly room temperature (~ 295 K). Density is less temperature dependent than

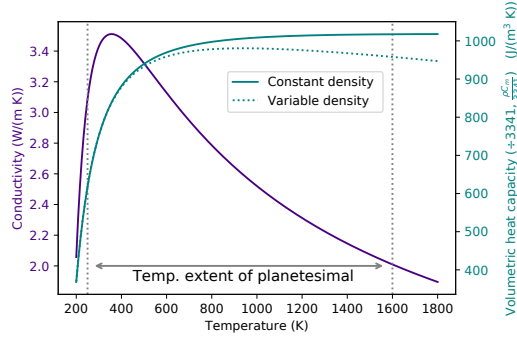


Figure 1. Temperature dependent material properties of olivine. As the temperature dependence of density (ρ) is small, heat capacity (C) and density are combined as volumetric heat capacity and are shown with a constant and T -dependent ρ to highlight the effect; both are divided by the value of the constant density, $\rho_0 = 3341 \text{ kg m}^{-3}$. These experimental functions are discussed further in section 2. Data from: Fei (2013); Robie et al. (1982); Su et al. (2018); Suzuki (1975); Xu et al. (2004).

C or k , and is combined with heat capacity in Figure 1 as volumetric heat capacity, both as a constant and as a T -dependent function to illustrate the scale of its effect.

Previous models of planetesimal thermal evolution take various approaches to the incorporation of k , ρ and C . These models address different stages of planetesimal evolution, depending on the meteorite group of interest, and can be broadly grouped into two classes. Models focusing on the accretion, early heating and melting of asteroids and planetoids investigate the origin of primitive meteorites (Allan & Jacobs, 1956; Elkins-Tanton et al., 2011; Hevey & Sanders, 2006), while conductive cooling models examine the post-peak- T period following recrystallisation and capture the genesis of extensively differentiated meteorites such as pallasites (Bryson et al., 2015; Ghosh & McSween, 1999; Haack et al., 1990; Tarduno et al., 2012). Models in the first class, for example those investigating the ordinary chondrite parent body, often employ temperature-dependent diffusivity from Yomogida and Matsui (1983): $\kappa = A + B/T$, where A and B are terms that describe the degree of compaction of the parent body (Akridge et al., 1998; Bennett & McSween, 1996; Harrison & Grimm, 2010). Ghosh and McSween (1999) highlight the importance of incorporating a temperature-dependent specific heat capacity in the modelling of primitive asteroids, recording a decrease in peak temperatures and corresponding change in closure temperatures when T -dependent C is used, but hold k and ρ constant.

The second class of models, which address conductive cooling in differentiated planetesimals such as the primary pallasite parent body (Bryson et al., 2015), generally assume k , ρ and C are independent of temperature. When experimentally investigating the effect of Fe content on olivine conductivity, Zhang et al. (2019) comment on the inclusion of T -dependent and composition-dependent k in their COMSOLTM models and note that the inclusion of variable properties have a non-negligible effect on the thermal evolution of a silicate sphere. However, the focus of the study is olivine forsterite content and the impact of olivine composition on the thermal evolution of planetary bodies, and T -dependence is not systematically explored. The implications of neglecting T -dependent k , ρ and C on the interpretation of meteorite parent body models is not understood.

The pallasite parent body has been chosen as an example for this study as previous research has tied paleomagnetism identified in meteorite samples to the period of core crystallisation in the parent body (Bryson et al., 2015; Tarduno et al., 2012). In order for the metal portion of a pallasite meteorite to record a convectional core dynamo, it must cool through the Curie temperature of its metal portion while the core is crystallising. Modifying the material properties of the body affects whether this condition is met. This places an easily-testable constraint on models to investigate the importance of including T -dependent properties when deciding parent body geometry, the formation depth of pallasite meteorites, and the number of parent bodies required.

Before we address the specific example of the pallasite parent body, we outline the approach used to incorporate T -dependent properties in models of conductive cooling of planetesimals and show how, even in simple cases, this can have an important influence on their thermal history. We first address the model and numerical scheme in section 2, before exploring the sensitivity of the model to different parameters with k , C and ρ as independent of T and investigating the range of parameters used in the literature. We then address the incorporation of a non-linear term when T -dependent k is included by using a series of simple linear functions for $k(T)$ in section 3.2. We implement T -dependent functions for k , C and ρ in section 3.3, and attempt to recreate these results by averaging the values for k , C and ρ radially and through time and then using these mean values in the constant model. Finally, we discuss the relevance to modelling the pallasite parent body.

2 Methods

To investigate the effect of including temperature-dependent properties in the thermal evolution of planetesimals, we used the 1D in radius r heat conduction equation with a non-linear term to allow for temperature dependence of k , ρ and C (Carslaw & Jaeger, 1986; Özisik, 1993). As in Bryson et al. (2015), the layered body is composed of three primary materials: a metallic FeS core which is initially molten, a solid olivine mantle and an insulating regolith layer (see Figure 2). Assuming a purely conductive mantle following magma-ocean solidification, in which convective heat transport is neglected, the temperature T in the mantle satisfies the differential heat conduction equation in spherical geometry:

$$\frac{\partial T}{\partial t} \rho C = \frac{1}{r^2} \frac{\partial}{\partial r} \left(kr^2 \frac{\partial T}{\partial r} \right) = \overbrace{\frac{dk}{dT} \left(\frac{\partial T}{\partial r} \right)^2}^{\text{non-linear term}} + \underbrace{\frac{2k}{r} \frac{\partial T}{\partial r}}_{\text{geometric term}} + \overbrace{k \frac{\partial^2 T}{\partial r^2}}^{\text{linear term}}, \quad (1)$$

where t is time. The non-linear term arises due to the T -dependence of k . The insulating regolith layer is given a constant diffusivity lower than that of the mantle as in Bryson et al. (2015). Pressure and self-gravitation are not incorporated into the current model. The boundary and initial conditions are chosen as follows:

$$T(r_p, t) = T_{\text{surf}}, \quad T(r, t_0) = T_{\text{init}}, \quad T(r_c, t) = T_c(t), \quad (2)$$

where r_p is the planetesimal radius, r_c is the core radius, T_{surf} is the constant surface temperature, T_c is the core temperature and T_{init} is the initial temperature, implying an homogeneous initial interior temperature distribution at t_0 ; the code can accommodate a heterogeneous initial temperature array but this is not used in this study. A Dirichlet boundary condition has been applied to the surface as in Bryson et al. (2015) instead of a radiative condition as used by Ghosh and McSween (1998), assuming the temperature at the surface of the planetesimal is constant and that of the ambient Solar nebula. While a radiative boundary condition is a closer approximation to the physical sys-

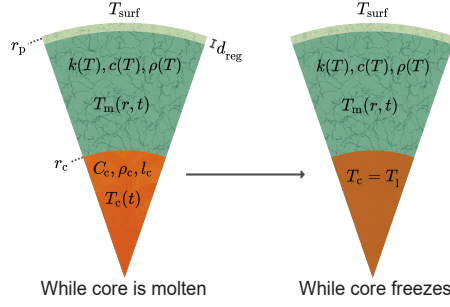


Figure 2. Not to scale. General model set-up, both before and during core solidification, displaying the functions relevant to different regions. Core radius is defined as a fraction of the total planetary radius, which includes the regolith layer. The regolith has a constant κ .

tem, a simpler fixed-temperature boundary condition has been found to produce negligible difference in inner-Solar System asteroidal models (Hevey & Sanders, 2006; Moskovitz & Gaidos, 2011).

The boundary condition for the base of the mantle depends on the core temperature. The core is assumed to be entirely liquid and vigorously convecting when molten (Bryson et al., 2015; Tarduno et al., 2012). The core temperature is updated by considering the total energy extracted across the core-mantle boundary (CMB). The energy transferred during a small time increment δt is

$$E_{\text{CMB}} = -A_c k_{\text{CMB}} \left. \frac{\partial T}{\partial r} \right|_{r=r_c} \delta t, \quad (3)$$

where A_c is the surface area of the core, r_c is the radius of the core, and k_{cmb} is the thermal conductivity at the base of the mantle at the CMB, i.e. $k_{\text{CMB}} = k_m(T(r_c, t))$. As $E_{\text{CMB}} = \rho_c V_c C_c \Delta T$ where V_c is the total volume of the core and ΔT is change in temperature, the change in the core temperature in one time increment (ΔT_c) is:

$$\Delta T_c = \frac{A_c k_{\text{CMB}} \left. \frac{\partial T}{\partial r} \right|_{r=r_c} \delta t}{\rho_c C_c V_c} = \frac{3 k_{\text{CMB}} \left. \frac{\partial T}{\partial r} \right|_{r=r_c} \delta t}{\rho_c C_c r_c}. \quad (4)$$

The temperature at the base of the mantle is then updated by adding ΔT to the temperature at the previous timestep:

$$T_{\text{CMB}}(r_c, t) = T_{\text{CMB}}(r_c, t - \delta t) + \Delta T_c. \quad (5)$$

The core cools as the mantle conducts heat to the surface, and is assumed to solidify when T_c reaches the melting temperature of the FeS core (T_l , in this case $T_l = 1200$ K, Bryson et al. (2015)). Once the core begins to freeze, the temperature is constant at T_l as latent heat is extracted across the CMB. The liquid and solid fraction act identically during this process and partitioning of elements is not addressed during freezing. The core solidifies entirely once the total latent heat associated with crystallisation has been extracted — when E_{CMB} during the solidification period exceeds E_l , where the total latent heat of the core is:

$$E_l = m_c L_c = \frac{4}{3} \pi r_c^3 \rho_c L_c, \quad (6)$$

where m_c is the mass of the core and L_c the specific latent heat of fusion of the core (Bryson et al., 2015; Tarduno et al., 2012).

2.1 Numerical Implementation

We solve the conduction equation numerically for the mantle using an explicit finite difference scheme with first order differences in time and second order in space. Equation 1 can be rewritten with the temperature at radius r and time t denoted by T_r^t :

$$T_r^t = T_r^{t-\delta t} + \frac{1}{\rho C} \delta t \times \left(\underbrace{\left. \frac{dk}{dT} \right|_r^{t-\delta t} \frac{(T_{r+\delta r}^{t-\delta t} - T_{r-\delta r}^{t-\delta t})^2}{4\delta r^2}}_{\text{non-linear term}} + \underbrace{\frac{k}{r\delta r} (T_{r+\delta r}^{t-\delta t} - T_{r-\delta r}^{t-\delta t})}_{\text{geometric term}} + \underbrace{\frac{k}{\delta r^2} (T_{r+\delta r}^{t-\delta t} - 2T_r^{t-\delta t} + T_{r-\delta r}^{t-\delta t})}_{\text{linear term}} \right), \quad (7)$$

where δt and δr are the constant timestep and radius step, and k is evaluated at $T_r^{t-\delta t}$. A consequence of this discretisation is that temperature dependent properties lag if evaluated at $t - \delta t$. A more accurate method is to evaluate k as

$$k^t = k^{t-\delta t} + \left(\frac{\partial k}{\partial T} \right)^{t-\delta t} (T^{t-\delta t} - T^{t-2\delta t}), \quad (8)$$

and similarly for C and ρ (Özışık, 1993). To reduce the error associated with variable k not being centred in time, we chose a sufficiently small δt such that $k(T_r^{t-\delta t}) \approx k(T_r^t)$, within a defined error ($< 1\%$ of k). We compared this with a selection of runs using the more accurate but computationally expensive method above for k^t and $C\rho^t$, and the differences in results were negligible. The maximum timestep allowable for stability in this numerical method must satisfy Von Neumann stability criteria, discussed in the supplementary information. This numerical solution, with constant k , C and ρ , was compared with an analytical solution from Crank (1979) which is also described in the supplementary information.

2.2 Meteorite formation depth

To illustrate the implications of this study on the pallasite parent body, we calculate the formation depths of pallasite meteorite samples, Imilac and Esquel, using the method and recorded cooling rates of Bryson et al. (2015). The FeNi portion of pallasite meteorites records the cooling rate of the sample at 800 K (J. Yang et al., 2010). The intersection between the cooling rate contour and the 800 K isotherm gives a formation depth. Then, the time when this depth passes through the tetrataenite formation temperature (593 K) and is magnetically recording can be compared to the timing of core crystallisation to see if it occurs while the core is freezing, thus potentially recording core dynamo activity (Bryson et al., 2015).

2.3 Parameter choices for the pallasite parent body

We selected parameters from previous models of planets, planetesimals and asteroids in the literature and experimental results from geochemistry and mineral physics studies as detailed in Table 1. For many of these parameters, we have chosen both a reference value relevant to our example case of the pallasite parent body, and a range of values used in other models of differentiated planetesimals with different assumptions regarding geometry and composition. Reference values related to the geometry of the planetesimal, the core, the boundary conditions and the calculation of meteorite formation depth recreate the model of Bryson et al. (2015), while mantle olivine properties have been chosen from experimental results (Table 1) as Bryson et al. (2015) use a constant κ . While Bryson et al. (2015) use a planetesimal radius $r_p = 200$ km, we have chosen

Table 1. *Model Parameters.*

Symbol	Parameter	Value(s)	Units
r_p	Planetesimal radius	250 , 150 – 600 ^{b,d,s}	km
r_c	Core radius	50 ^{b,s} , 20 – 80 ^q	% of r_p
d_{reg}	Regolith thickness	8 ^b , 0 – 20 ^{i,t}	km
k	Mantle conductivity	3 ^b , 1.5 – 4 ^{e,w,aa}	W m ⁻¹ K ⁻¹
C	Mantle heat capacity	819 ^r , 600 – 2000 ^{h,k,n,o,s}	J kg ⁻¹ K ⁻¹
ρ	Mantle density	3341 ^r , 2500 – 3560 ^{l,m,y}	kg m ⁻³
C_c	Core heat capacity	850 ^{p,z} , 780 – 850 ^{c,u}	J kg ⁻¹ K ⁻¹
ρ_c	Core density	7800 ^o , 7011 – 7800 ^{c,l,p,u}	kg m ⁻³
κ_{reg}	Regolith diffusivity	5 × 10⁻⁷ ^b	m ² s ⁻¹
L_c	Latent heat of fusion of core	2.7 × 10⁵ ^{g,o} , 2.56 × 10 ⁵ ^p	J kg ⁻¹
T_l	Freezing temperature of core	1200 ^b , 1213 ^{g,o,s}	K
T_{init}	Initial temperature	1600 ^b , 1450 – 1820 ^{o,p}	K
T_{surf}	Surface temperature	250 ^{j,v} , 150 – 300 ^{a,f,o}	K
T_{cz}	Tetrataenite formation temp.	593 ^b	K
T_{cr}	Cooling-rate temperature	800 ^{b,x}	K
δt	Timestep	1 × 10 ¹¹	s
δr	Radial step	1000	m

Note: Reference values in **bold**. ^a Boss (1998), ^b Bryson et al. (2015), ^c Davies and Pommier (2018), ^d The OSIRIS-REx Team et al. (2019), ^e Elkins-Tanton et al. (2011), ^f Gail et al. (2014), ^g Ghosh and McSween (1998), ^h Ghosh and McSween (1999), ⁱ Haack et al. (1990), ^j Hevey and Sanders (2006), ^k Hort (1997), ^l Johnson et al. (2019), ^m Miyamoto et al. (1982), ⁿ Robie et al. (1982), ^o Sahijpal et al. (2007), ^p Scheinberg et al. (2015), ^q Solomon (1979), ^r Su et al. (2018), ^s Tarduno et al. (2012), ^t Warren (2011), ^u Williams and Nimmo (2004), ^v Woolum and Cassen (1999), ^w Xu et al. (2004), ^x C. W. Yang et al. (1997), ^y Yomogida and Matsui (1983), ^z Young (1991), ^{aa} Zhang et al. (2019).

$r_p = 250$ km as our reference value so that paleomagnetic recording occurs while the core is crystallising for both samples (section 2.2).

Initially, we allowed models to run for 400 million years. We increased the run time if it did not capture the period of core solidification, for example in cases with larger radii. The core reverts to an isothermal state following the solidification period. This simplified approximation of a highly-conductive metallic core is sufficient for the example application in this study, for which the post core-solidification period is not of interest.

2.4 Incorporation of temperature dependent properties

For this study, we have chosen the function used for heat capacity in olivine at ambient pressures from Su et al. (2018), based on lattice vibration theory from Berman and Brown (1985) and fit to experimental data from Isaak (1992):

$$C = 995.1 + \frac{1343}{\sqrt{T}} + \frac{2.887 \times 10^7}{T^2} - \frac{6.166}{T^3}. \quad (9)$$

Note that this is valid for the range of temperatures $T_{\text{surf}} - T_{\text{init}}$. We don't explore temperatures close to 0 K. The expression for thermal expansivity is also taken from Su et

al. (2018) based on the functional fit by Fei (2013) and using experimental data from Suzuki (1975):

$$\alpha = 3.304 \times 10^{-5} + 0.742 \times 10^{-8}T - 0.538T^{-2}. \quad (10)$$

As described in section 1, α can be used to calculate the change in density with temperature: $\rho = \rho_0 - \alpha\rho_0(T - T_0)$, where $T_0 = 295$ K and $\rho_0 = 3341$ kg m⁻³.

As the lower temperatures modelled (~ 250 K) are rarely of interest in terrestrial mineral physics and are less accessible to experimental studies, we constructed a simple conductivity function for olivine spanning 250 – 1800 K. As discussed in section 1, conductivity is controlled by different process at high and low temperatures, resulting in different temperature dependencies. For the high- T region, we used the experimentally-derived curve from Xu et al. (2004):

$$k = 4.13 \times \left(\frac{298}{T} \right)^{\frac{1}{2}} \times (1 + aP), \quad (11)$$

where $a = 0.032$ GPa⁻¹ (experimentally derived) and $P = 4$ GPa. As T -dependence of k at temperatures $\ll \theta_D$ is similar to that of C , a function identical in shape to equation 9 but normalised such that $C = 1$ at $T > \theta_D$ was used for the low- T region. As this low- T curve is constant and equal to 1 above θ_D , it can be multiplied by equation 11 to fill in the low- T region without altering the higher- T experimental results. Our resultant function is differentiable and non-monotonic:

$$k = 80.421 \times \left(1.319 \times T^{-\frac{1}{2}} + 0.978 - \frac{28361.765}{T^2} - \frac{6.057 \times 10^{-5}}{T^3} \right) \times T^{-\frac{1}{2}}, \quad (12)$$

While the pressures inside the planetesimal are $\ll 4$ GPa, changing pressure to < 1 GPa in equation (11) increases conductivity in our composite function by < 0.3 W/(m K) at all temperatures. As this is outside of the calibration range of the experiments by Xu et al. (2004) we have chosen not to include this adjustment as it may not be physically realistic and pressure effects are not the focus of this study, and instead use a and P as quoted by Xu et al. (2004). These functions are illustrated in Figure 1.

In order to fully understand the effect of including temperature dependence in our model, we also constructed a simple linear function for conductivity before investigating the more complex equation (12):

$$k = k_0 + \beta T, \quad (13)$$

where k_0 is a reference conductivity at 0 K and β controls the temperature dependence, and can be set as positive or negative. β and k_0 must be chosen such that k does not become negative over the temperatures explored in the body. In order to contrast a T -dependent conductivity with simply setting the average conductivity higher or lower, functions with both positive and negative β were chosen to approximate the same mean conductivity over radius and time. Additionally, the cases were run with and without the non-linear term. Both ρ and C were held constant to isolate the effect of the conductivity. The regolith layer maintains a constant κ for all model runs including those with fully variable k , ρ and C , as after initial rapid equilibration with the surface temperature, this layer has a constant temperature. The core properties have also been kept constant.

3 Results

The model produces arrays of temperature and cooling rate through time and radius. For any radius r , the linear, geometric and non-linear (if applicable) terms of the heat conduction equation can be plotted against time. Model outputs that are important to the interpretation of meteorites include the initiation and duration of core crystallisation, the depth within the parent body from which the meteorite was derived and when this occurred, and the peak cooling rates reached. In the specific case of the palasite parent body, the calculated depth of formation can then be tracked to see if this region of the parent body passes through the temperature where magnetism is recorded while the core is solidifying, thus potentially recording core dynamo activity.

3.1 Constant k , ρ and C

The model was run with constant k , ρ and C for both the reference parameters in table 1 and the end-member values quoted, if applicable. In addition, parameters were varied by $\pm 10\%$ of the reference value to gauge the sensitivity of the model to different inputs. The full results of these parameter explorations are tabulated in the supplementary information.

Figure 3 shows the chosen reference case for the constant k , ρ and c . The linear term initially dominates the cooling, especially in the shallower regions of the body where there is lower curvature (Figure 3a); the geometric term that accounts for the body's spherical geometry is of more relative importance deeper within the body at smaller radii (Figure 3b). Peak cooling rates are higher and are reached marginally earlier in the shallow portion of the body, as the near-surface rapidly equilibrates with the boundary held at 250 K while the temperature anomaly propagates through the mantle to deeper regions with a time delay determined by the diffusion timescale.

The slope of $T(r)$ from the base of the mantle to the surface is negative for the duration of the model run. Initially, $T(r)$ is convex upwards but flattens over time and becomes convex downwards as the linear term changes sign: initially within the body $\frac{\partial^2 T}{\partial r^2}$ is negative for all radii and increases with time, becoming positive at the boundaries first, with this change in sign propagating towards the middle of the mantle. When the core is removed to approximate a solid sphere, this effect is only seen to propagate downwards from the surface boundary as the breaking effect of the core on the cooling of the mantle is not present. The geometric term then drives further cooling after this point (Figure 3).

When the core reaches 1200 K and begins to freeze, the temperature at the CMB is held constant. The fixed core temperature reduces the cooling rate in the mantle sharply; in the deeper regions of the mantle $-\frac{\partial T}{\partial t}$ drops towards zero as the mantle reaches the same temperature as the core. The effect is less pronounced in the shallow regions as the cooling rate has already slowed significantly and is approaching zero.

The body cools rapidly at the surface, with shallow depths quickly equilibrating with the constant surface temperature (Figure 4). High temperatures are maintained for longer deeper within the body due to the overlying insulating mantle. Using the cooling rates calculated by Bryson et al. (2015), we calculated source depths of 64 km for Esquel and 57 km for Imilac, approximately midway through the mantle (Figure 4 and Table 2).

The geometry of the body is a strong controlling factor on the cooling rate and timing of core crystallisation (Table 2). The planetary radius has the largest effect: increasing the total radius by 10 % slows the cooling of the planetesimal at depth and delays the onset of core crystallisation by 38 Myr. When the core fraction is increased, the core begins to freeze 5 Myr earlier as there is less insulating mantle, but takes 4 Myr longer

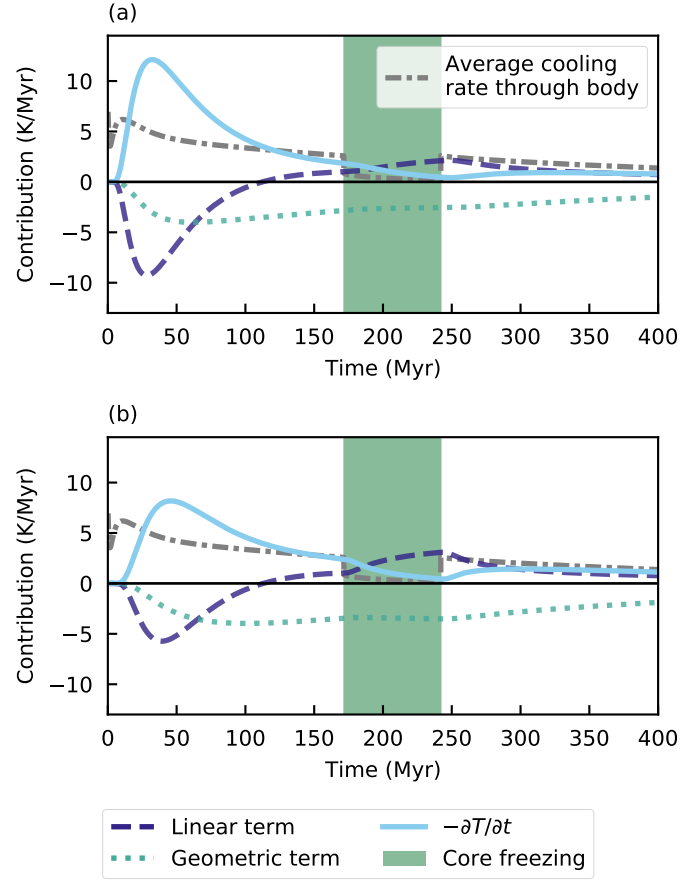


Figure 3. Results for the reference case with constant k , ρ and C . The components of the heat conduction equation are shown at a depth of (a) 42 km (one third of the thickness of the mantle) and (b) 84 km (two thirds). The cooling rate is multiplied by -1 to illustrate how it balances the other components to add to zero. The shaded green area defines the period of core crystallisation.

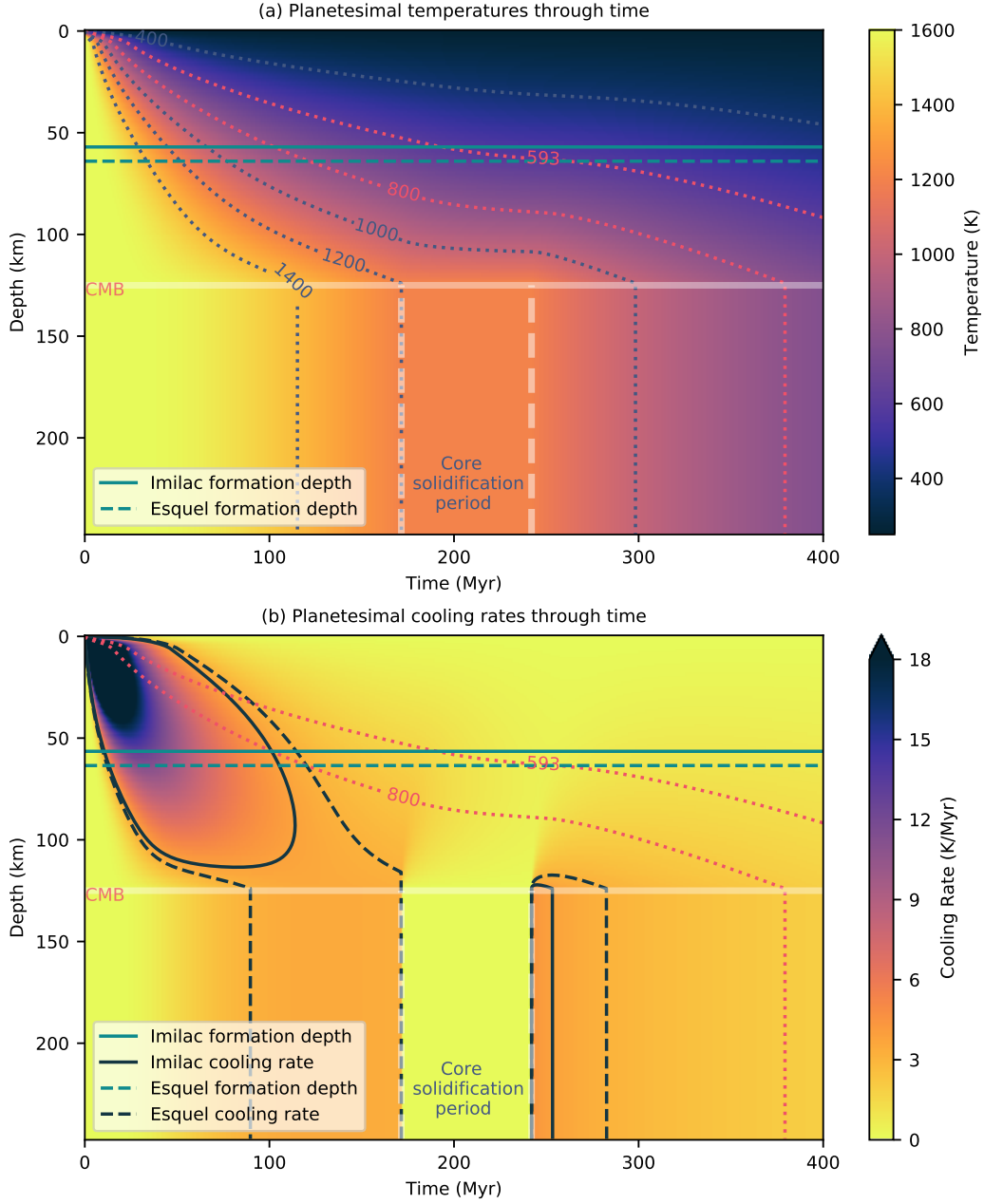


Figure 4. Planetary (a) temperatures and (b) cooling rates through time for the default model with constant k , ρ and c . The calculated source depth of the Imilac and Esquel meteorites for this model set-up are shown in both plots, using the cooling rate data and method of Bryson et al. (2015). Temperature contours highlight the tetrataenite formation temperature when paleomagnetism can be recorded (593 K) and the temperature for which the sample's cooling rates were measured (800 K), while cooling rate contours show the measured cooling rates for both samples.

Table 2. *Model results for constant k , ρ and C*

Varied parameter	Value	Core starts Myr	Core ends Myr	Duration Myr	Esquel depth km	Imilac depth km
Reference case		172	242	70	64	57
$r_p + 10\%$	275 km	210	296	86	64	56
$r_c + 10\%$	138 km	167	241	74	58	53
$r_{\text{reg}} + 1 \text{ km}^a$	9 km	172	242	71	64	57
$k + 10\%$	$3.3 \text{ W m}^{-1} \text{ K}^{-1}$	157	221	64	68	60
$C + 10\%^b$	$901 \text{ J kg}^{-1} \text{ K}^{-1}$	180	252	72	61	54
k_{max}	$4 \text{ W m}^{-1} \text{ K}^{-1}$	132	185	53	77	67
k_{min}	$1.5 \text{ W m}^{-1} \text{ K}^{-1}$	330	400	70	42	36

Note: Model results with parameters varied to $\pm 10\%$ of the default value, with endmember cases included for k . References for parameter choices given in Table 1. ^aRegolith thickness was increased and decreased by 1 km as 10 % (0.8 km) is smaller than δr .

^bIncreasing or decreasing C or ρ (not both) by 10 % results in a change in ρC by 10 %. Full results in supplementary information.

to freeze fully due to its increased size. While the average cooling rate of the body drops sharply for all cases on initiation of core solidification, the effect is more pronounced when the core fraction is increased as the cooling rate of the core dominates the overall cooling rate. Increasing the insulating regolith thickness by 1 km while maintaining a 250 km total radius does not delay the onset of core crystallisation, but does increase the duration of the solidification period by 1 Myr. Increasing the regolith thickness further does delay core solidification, with a 20 km thick regolith causing a 73 Myr delay when compared to the reference case (see supplementary information). The resulting changes in the calculated source region depth for pallasite meteorites is also shown in Table 2.

Increasing k by 10 % accelerates the cooling in the body, causing the core to begin solidifying 15 Myr earlier. Increasing ρ or C by 10 % has the opposite effect, and delays the onset of core crystallisation by 8 Myr. Table 2 also shows the results of setting $k = 4 \text{ W m}^{-1} \text{ K}^{-1}$ and $1 \text{ W m}^{-1} \text{ K}^{-1}$, which reflect the end-member expected values if k varied with T (see Figure 1). Between these two cases, there is a 198 Myr difference in the timing of the start of core solidification. The core begins to freeze at 132 Myr and the freezing period lasts 53 Myr when $k = 4 \text{ W m}^{-1} \text{ K}^{-1}$, while the core begins to freeze at 330 Myr when $k = 1 \text{ W m}^{-1} \text{ K}^{-1}$. An increase in conductivity results in deeper source regions for the pallasite meteorites, with the Esquel and Imilac source regions moving 13 and 10 km deeper respectively when $k = 4 \text{ W m}^{-1} \text{ K}^{-1}$, while both move ~ 22 km shallower when $k = 1 \text{ W m}^{-1} \text{ K}^{-1}$.

3.2 Simple linear T -dependent conductivity

In this section we explore $k(T)$ in the form $k = k_0 + (\beta T)$ with ρ and C held constant. For the examples shown in Figure 5 and summarised in table 3, we chose $\beta = \pm 0.0025 \text{ W/(m K}^2\text{)}$ and k_0 such that $k = 3.0 \text{ W/(m K)}$ at the mean temperature of the reference case with constant k , ρ and c (with regolith thickness set to 0 km - Table 3) to isolate the effect of T -dependence. The model was run both with and without the non-linear term in Figures 5a and 5b). When compared to the constant case with $k = 3 \text{ W/(m K)}$, allowing k to vary with T changes the timing and duration of the core crystallisa-

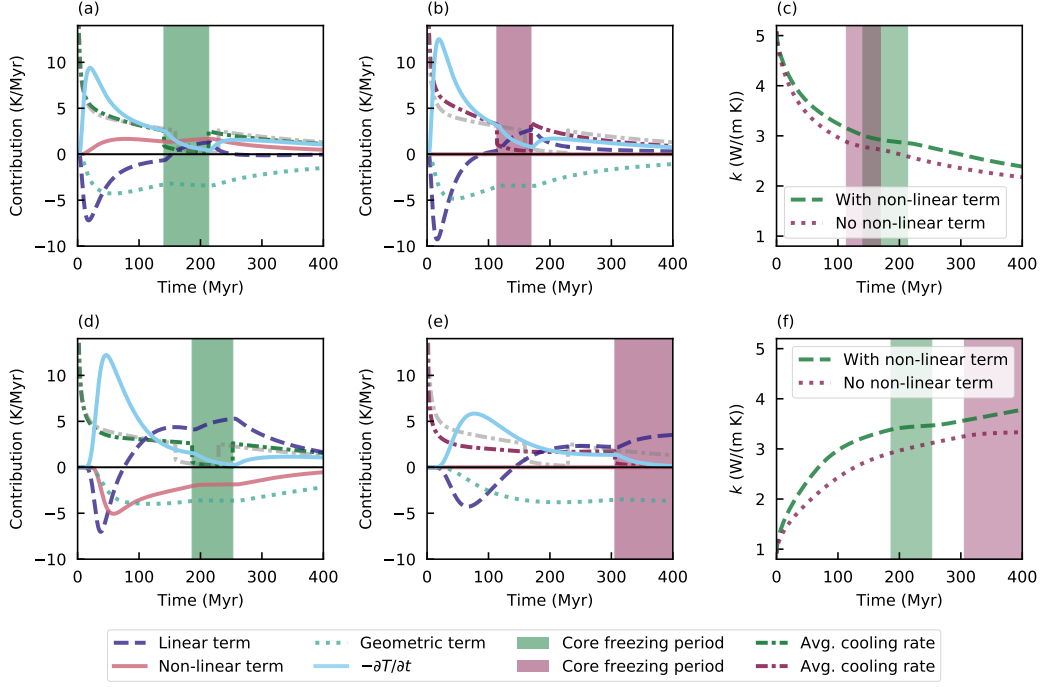


Figure 5. Results for model with a linear function for $k(T)$ and constant ρC . Panels (a), (b) and (c) show results for $\beta = 0.0025$. Panels (a) and (b) show the components of the heat equation with and without the non-linear term, with the cooling rate averaged across all radii included and compared to the reference case with 9 km regolith. Panel (c) shows the average conductivity through time for both these cases with the core crystallisation period highlighted. Panels (d), (e) and (f) show the equivalent results for $\beta = -0.0025$.

tion period (see table 3). For $\beta = 0.0025$ W/(m K²) and $k_0 = 1.1125$ W/(m K) (panel (a), Figure 5), the onset of core crystallisation is 19 Myr earlier than for the constant case (table 3); in the early stages of the model run the average cooling rate throughout the body is higher than the constant case due to higher initial conductivity in the mantle (panel (c) of Figure 5). After ~ 80 Myr (before the core begins to freeze), the average cooling rate throughout the body drops below the constant case, resulting in a 3 Myr longer core-crystallisation period. The duration of core crystallisation is close to that of the constant case as, during this time period, the variable conductivity is similar to the fixed conductivity of the constant case (panel (c), Figure 3).

When the non-linear term is neglected (panel (b), Figure 5), core crystallisation initiates 46 Myr earlier than in the constant reference case, due to increased cooling rates despite a lower average conductivity. The non-linear term is always positive and slows cooling if $\beta > 0$, reducing the peak cooling rates experienced at this depth and the average cooling rates in the mantle.

The equivalent results for $\beta = -0.0025$ are shown in panels (d), (e) and (f) of Figure 5 and in Table 3. For $\beta = -0.0025$ W/(m K²) and $k_0 = 4.8875$, the onset of core solidification is delayed by 27 Myr and the period of core crystallisation is 4 Myr shorter than for the constant case due to the increasing conductivity of the mantle. The non-linear term in this case is negative, owing to the negative sign of $\frac{dK}{dt}$, and it amplifies the initial peak cooling rates at the depth examined (panel (d), Figure 5); however, the overall average cooling rate of the body is initially lower due to the low con-

Table 3. *Simple linear function for conductivity*

Model	Slope β	Reference k_0	Average mantle k	Core starts solidifying	Duration of solidification
	W/(m K ²)	W/(m K)	W/(m K)	Myr	Myr
Constant case	0.00	3.00	3.00	159.24 ^a	70.17 ^a
Positive β	0.0025	1.1125	3.02	140.52	72.79
Positive β without non-linear term	0.0025	1.1125	2.77	113.62	55.40
Negative β	-0.0025	4.8875	3.16	186.37	66.11
Negative β without non-linear term	-0.0025	4.8875	2.76	305.73	94.27

Note: Model results with a linear function for k . Regolith thickness is set to 0 km in all cases.

^aAs regolith is not included, note the earlier solidification than for the reference case with 8 km regolith, where the core starts solidifying at 171.58 Myr and the solidification period lasts 70.43 Myr.

ductivity (Figure 5f). When the non-linear term is neglected, the core begins to solidify 146 Myr later than in the constant case, and solidification takes 24 Myr longer. As the core does not freeze at the midpoint between the initial and surface temperatures, the non-linear terms for positive and negative β are not symmetric.

In summary, positive β leads to earlier onset of core freezing and a longer duration of core freezing, while negative β results in later onset of freezing and a shorter freezing period. For both $\pm\beta$ the change in onset time when compared to the constant case is much larger than the change in the duration of core freezing, as there is a much greater difference between constant and variable k earlier in the model than during core solidification (Figures 5c, 5d). Even for linear conductivity functions with shallow slopes, the conductivity structure of the mantle is very different to that of the constant case and the temporal dependence of this structure has implications for the timing of events within the body that cannot be approximated by changing the value of k in the constant case. Inclusion of the non-linear term is essential as neglecting it can result in large over- or underestimations of core crystallisation onset time (for negative β , neglecting the non-linear term results in 119 Myr delay in the onset of core crystallisation). The implications of these results on the pallasite parent body are investigated using the experimentally derived functions in the next section.

3.3 Temperature-dependent properties: using experimental functions

The fully variable case, using the default parameters in Table 1 and the $k(T)$, $C(T)$ and $\rho(T)$ functions (equations 9, 10 and 12), resulted in a 40 Myr delay in the onset of core crystallisation but only 3 Myr longer period of core crystallisation when compared to the reference case with constant properties (Figure 6). The temperature distribution in the shallow mantle is similar to that of the constant reference case, but the interior stays hotter for longer when T -dependent properties are used (Figure 6). The fully variable case requires deeper source regions for the pallasite meteorite samples than the reference case, with a depth of 61 km calculated for Imilac and 68 km for Esquel (Table 4).

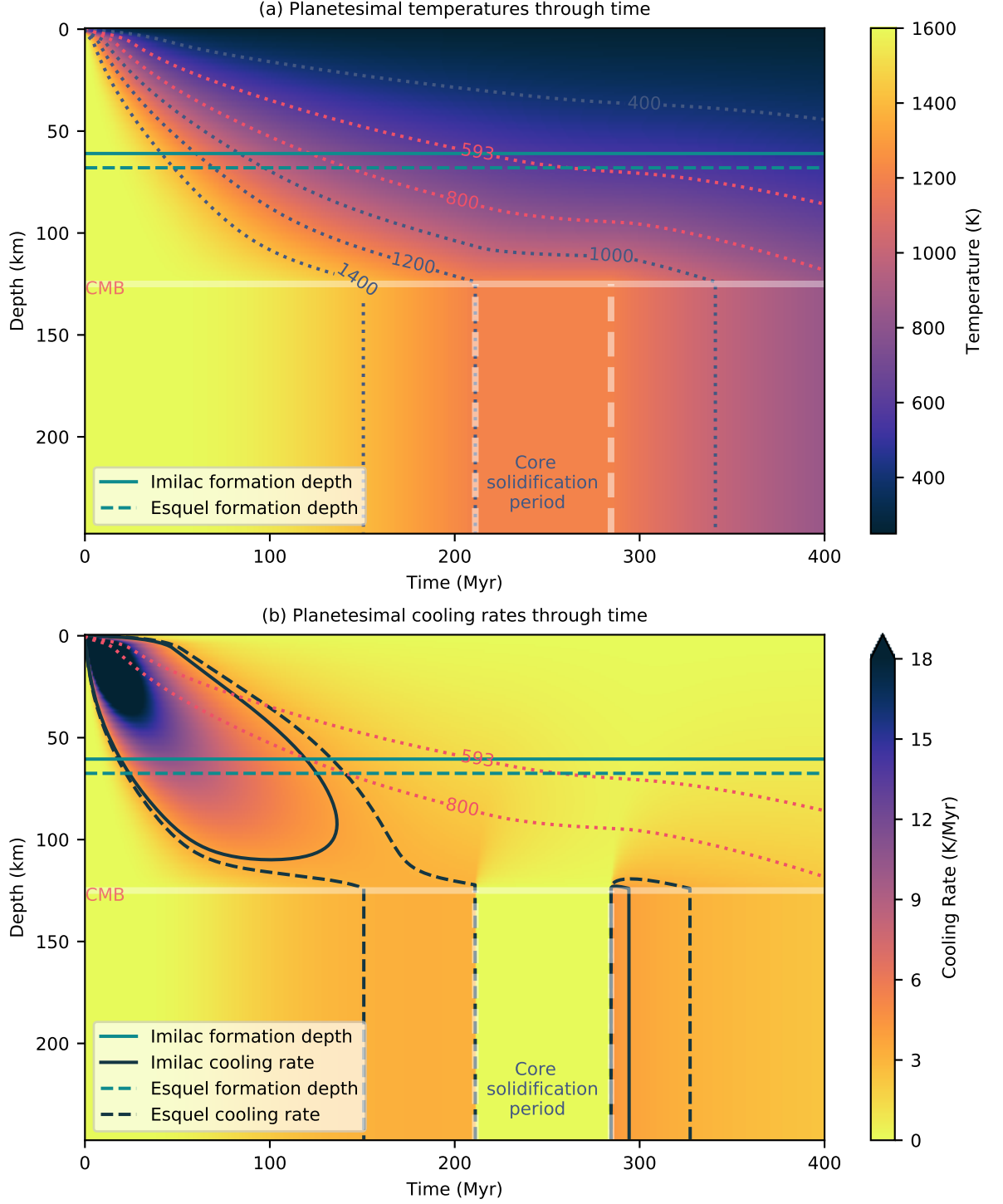


Figure 6. Planetesimal (a) temperatures and (b) cooling rates through time for a model with T -dependent k , ρ and c . The calculated source depth of the Imilac and Esquel meteorites for this model set-up are shown in both plots, using the cooling rate data and method of Bryson et al. (2015). Temperature contours highlight the tetrataenite formation temperature when paleomagnetism can be recorded (593 K) and the temperature that corresponds to the sample's measured cooling rates (800 K), while cooling rate contours show the measured cooling rates for both samples.

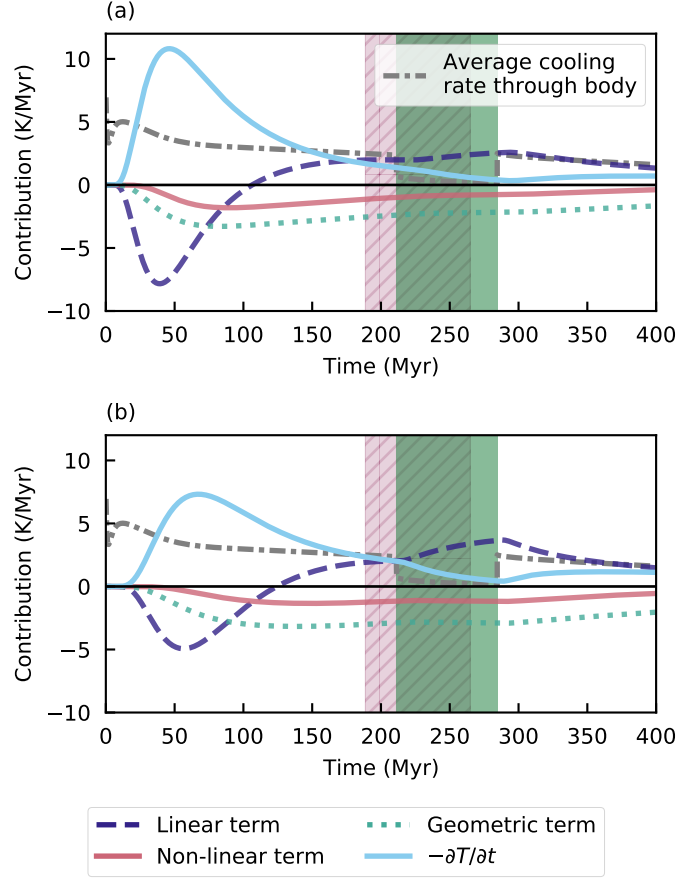


Figure 7. Results for the reference case with T -dependent k , ρ and C . The components of the heat conduction equation are shown at a depth of (a) 42 km (one third of the thickness of the mantle) and (b) 84 km (two thirds). The cooling rate is multiplied by -1 to illustrate how it balances the other components to add to zero. The green area defines the period of core crystallisation when T -dependent properties are used, while the pink area highlights the period of core crystallisation from the mean constant case for comparison.

When discussing simple linear functions for $k(T)$, we have demonstrated that cases with constant and variable properties should be correctly calibrated in order to make meaningful comparisons. In order to do so, we measured the average temperature in the mantle of the fully variable case and used this to calculate new constant values of k , C and ρ using equations 9, 10 and 12. The mean temperature of the mantle over the 400 Myr of the model lifetime was 780 K, giving $k = 2.8$ W/(m K), $\rho = 2945$ kg/m³ and $C = 996$ J/(kg K). The model with constant properties was then rerun with these updated values for k , ρ and C , to more closely approximate the results from the fully variable model. In this section, this new model using updated constant k , ρ and C is referred to as the constant mean values case, and the results are shown in table 4.

In the fully variable case (Figure 7), the non-linear term is negative and enhances the overall cooling rate at the depths displayed for all times shown (up to 400 Myr), as the slope of the function for k is negative for all $T > 300$ K (Figure 1). A thin insulating layer in the shallow mantle forms where $T < 300$ K and the non-linear term is positive. The core begins to freeze 211 Myr after model initiation, and takes 61 Myr to

Table 4. *Variable k , ρ and c .*

Model	Core Starts Myr	Core Stops Myr	Imilac depth km	Esquel depth km	Imilac timing Myr	Esquel timing Myr
Reference (constant k, ρ, c) ^a	172	242	57	64	185	240
Constant (mean k, ρ, c) ^b	189	265	53	60	186	226
Variable ^c	211	285	61	68	206	248
Variable (non-linear = 0) ^d	245	335	47	54	190	234
Variable conductivity ^e	200	272	64	71	206	260
Variable heat capacity ^e	190	266	53	60	186	226
Variable density ^e	198	276	50	57	185	224

Note: Summary of key results. Timing of core crystallisation period given in millions of years after model start (myr) and formation depth of meteorites given in km. ^aReference case with constant $k = 3 \text{ W m}^{-1} \text{ K}^{-1}$, $\rho = 3341 \text{ kg m}^{-3}$ and $C = 819 \text{ J kg}^{-1} \text{ K}^{-1}$. ^bConstant case here differs from the reference case: values for k , ρ and c are calculated at the mean T in the fully variable case: $k = 2.8 \text{ W m}^{-1} \text{ K}^{-1}$, $\rho = 2945 \text{ kg m}^{-3}$, and $C = 996 \text{ J kg}^{-1} \text{ K}^{-1}$. ^cCase with T -dependent k , ρ and c . ^d T -dependent properties, but with non-linear term neglected. ^eOne property allowed to vary with T with other properties held at mean values as in ^b.

fully solidify. The constant mean values case does not replicate this result: with constant k , ρ and C , the core begins to solidify at 189 Myr and takes 53 Myrs to fully freeze (Table 4). In addition, the constant mean values case requires shallower source regions for the pallasite meteorites Imilac and Esquel: 53 and 60 km respectively (Table 4). Qualitatively, the fully variable case is similar to the case with linear k and negative β in section 3.2: the core begins to freeze later but takes a shorter time than the constant mean values case (Tables 3 and 4). When the non-linear term is set to zero, again the fully variable model behaves similarly to the $\beta < 0$ linear case (Table 4).

When the different properties are allowed to vary in turn, T -dependent C produces the smallest deviation in core crystallisation timing from the constant mean values case, as at high T (temperatures such as those experienced by the planetesimals prior to and during core crystallisation), C is approximately constant (Figure 1). Including variable ρ results in a 9 Myr delay in the onset and 2 Myr longer duration of core crystallisation in comparison to the constant mean values case, while including only variable k results in an 11 Myr delay in the onset and a 4 Myr shorter duration of core crystallisation. Variable ρ produces the shallowest meteorite source regions of the three properties while variable k produces the deepest (Table 4). Including just one T -dependent property cannot replicate the fully variable model.

4 Discussion and Conclusion

Including T -dependent thermal properties changes the temperature structure in the modelled planetesimal: predictions of mantle temperature can differ by 50 K over tens of millions of years even when the best estimates for constant k , ρ and C are used (Figure 8). This results in significant changes in the timing and duration of core crystallisation: the onset of core solidification is 22 Myr later, a delay of 12 %. We use the example of a pallasite parent body to illustrate these results: including T -dependent prop-

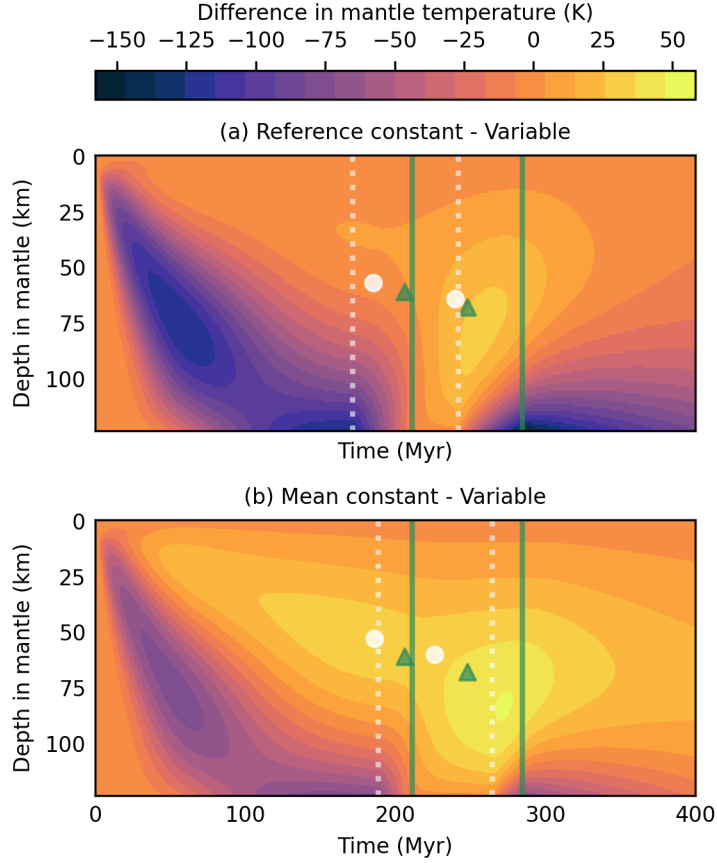


Figure 8. Difference in temperature distribution between (a) the reference constant model and variable model and (b) the mean constant model and variable model, where average k , ρ and C through time and radius are equal. Period of core crystallisation is shown in dashed white for the constant cases, and in green for the variable case. Symbols mark the source regions for the Imilac and Esquel meteorites as they pass through the 593 K isotherm; white circles show the results from the constant cases, while green shows the result when variable properties are used. Cooling rate data from Bryson et al. (2015)

erties delays the onset of core crystallisation and results in deeper source regions for pallasite meteorites than when constant k , ρ and C are used (Figure 8). In this example, T -dependent k , ρ and c result in a hotter deep mantle but cooler shallow mantle which cannot be replicated by constant values (Figure 8).

Including T -dependent properties also affects whether or not samples are predicted to preserve remnant magnetisation from a core dynamo: while in the constant reference case both the Imilac and Esquel meteorite source depths cool through 593 K during core freezing solidification, the Imilac region cools down below 593 K before core solidification when variable k , ρ and c or mean constant values based on the variable case are used (Table 4). While the relative timing of the meteorite source regions' cooling through 593 K and the core crystallising can be reproduced by the constant mean case for this example, the input values for k , ρ and C require the fully variable case to be run initially in order to be calculated.

In our example of a 250 km radius parent body, Imilac forms only ~ 5 Myr before the core begins to crystallise and so can be accounted for by error in the measurement of the cooling rate from this sample (from Bryson et al. (2015)). However, larger discrepancies in timing can be found for different cooling rates, parent body radii, regolith thickness or core fraction (Figure 9). Including T -dependent properties narrows the range of input parameters that allow meteorite samples to potentially record paleomagnetic signatures. This provides a simple criteria for testing different parameter combinations: whether the meteorite source region cools through the tetrataenite formation temperature during core solidification. As shown in Figure 9, when constant k , ρ and C are used, regolith thicknesses anywhere between 0 – 12 km satisfy the above criteria for a planetesimal of 250 km radius and a core that is 50% of r_p , while a regolith layer of 4 - 8 km is required when T -dependent properties are used. If the core fraction is reduced to 30% of r_p , a 250 km body with regolith between 0 - 8 km can accommodate both meteorite samples, whereas no suitable combination of parameters can be chosen when T -dependent k , ρ and c are used. Similarly, no suitable parent body with a 250 km radius and a core fraction of 70% r_p can be found if T -dependent properties are used, whereas if these values are taken as constant, then a planetesimal with a radius of 300 km including an 8 km thick regolith can produce the cooling rates and required timings in both meteorites.

One limitation of this work is the simplified core crystallisation model used. T -dependent properties have not been addressed for this region. Future work could develop or incorporate a more sophisticated core cooling and crystallisation model, to address issues such as directionality of crystallisation which may have implications for the interpretation of paleomagnetic signatures recorded in meteorite suites. Following crystallisation, the core is assumed to return to an isothermal state due to the high conductivity of the material. For the pallasite example case, this is an acceptable simplification as it is the times preceding and during the core solidification period that are of interest. For other applications it may be required to restart the model with the core included in the iterative solution with a Neumann boundary condition at the centre, as used for approximating the analytical solution (see Supplementary Information). The effects of pressure and gravity have also been neglected due to the low pressure gradient expected within the body as discussed in section 1.

In conclusion, T -dependent properties can significantly impact the output of planetesimal cooling models, even if the model results are being used qualitatively or to judge the relative timing of processes within the body, such as whether meteorite formation regions cool through specific temperatures before, during or after the period of core crystallisation. The inclusion of T -dependent k , ρ and C results in later crystallisation of the core (~ 40 Myr later than the constant reference case and ~ 20 Myr later than the updated constant case) and deeper meteorite formation depths due to suppressed cooling rates in the mantle. This result cannot be replicated with constant values for k , ρ and C , even when these values are chosen to match the mean values of each through time and

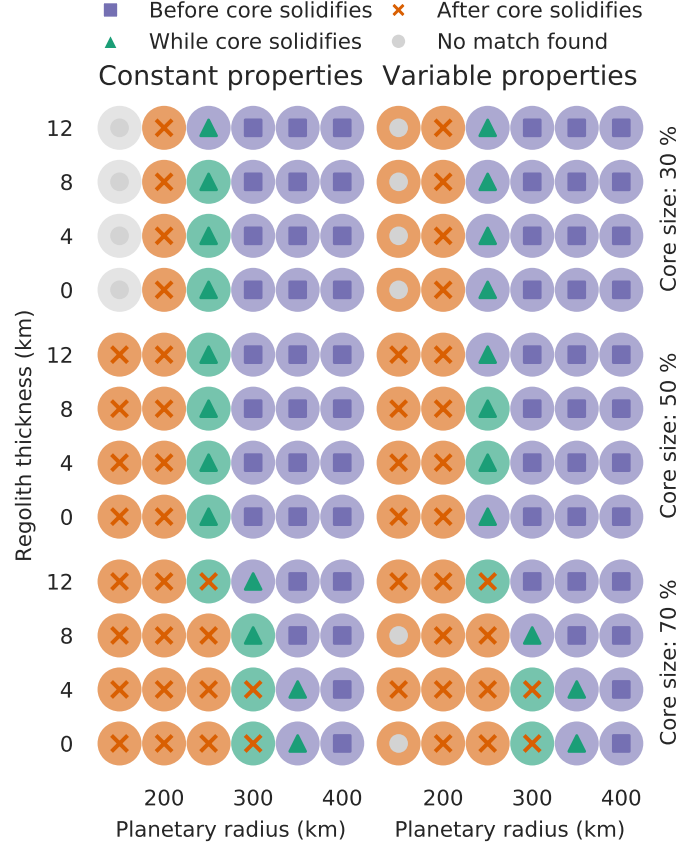


Figure 9. Planetary radius, core size and regolith thickness investigation for the constant k , ρ and C case, and the fully variable case. The small symbols represent the Esquel meteorite, while the larger circles represent Imilac. The colour and symbol denote whether or not the meteorite source region cooled through 593 K during core crystallisation ± 10 Myr: green circles or triangles mark models where this criteria was met. Red circles or crosses denote models where the meteorite cooled through 593 K after core crystallisation, whereas blue circles or squares show where this happened before the core began to crystallise. Grey markers note that no matches for the meteorite cooling rates at 800 K were found, implying the meteorite could not have formed in that body. Cooling rate data from Bryson et al. (2015).

radius in the variable model. If T -dependent κ is included without a non-linear term, the reduction in cooling rates through the body is overestimated, resulting in core solidification 33 Myr after the variable case and 73 Myr after the constant case. These results are shown with relevance to the pallasite parent body. The parameter space which satisfies the cooling rate criteria for the material which formed the Imilac and Esquel meteorites shrinks when T -dependent properties are included; it follows that if more samples are investigated the parameter space will shrink further. Future work could use this more restrictive parameter space to address the ongoing debate over the number of required pallasite parent bodies and potentially place a minimum constraint on the number of bodies required. T -dependent properties should also be addressed for other planetesimals and meteorite parent bodies where conduction is involved, for example the ordinary chondrite parent body, where peak temperatures and the inferred parent body radius may be incorrectly calculated.

Acknowledgments

Data availability: representative model output data are publically available from the National Geoscience Data Centre (NGDC), the Natural Environment Research Council (UK) data centre for geoscience data, under the ID 138605. Model is described in detail in the main text with all parameters used to allow for reproduction. MMQ was supported by the Leeds-York Natural Environment Research Council Doctoral Training Partnership (NE/L002574/1). CJD was supported by Natural Environment Research Council Independent Research Fellowship (NE/L011328/1).

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