

Interior Models of Mercury and Conditions for Iron Snow Formation in a Fe-S-Si Core



Key Points:

- The inner core radius and mantle density of Mercury sensitively depend on the normalized moment of inertia (MoI)
- A high MoI favors higher mantle densities and inner cores <1,100 km; a low MoI favors lower mantle densities and inner cores 850–1,450 km
- An iron snow layer in the liquid core requires a S concentration >2 wt%, inconsistent with core geochemistry

Supporting Information:

Supporting Information may be found in the online version of this article.

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Abstract Mercury's unique interior structure and magnetic field generation remain to be fully understood. We construct models to further constrain Mercury's interior and test the hypothesis that iron snow within the liquid core drives the dynamo. We build upon previous models by incorporating an updated iron-sulfur-silicon (Fe-S-Si) core alloy composition and use a Monte Carlo approach to explore the parameter space consistent with geodetic and geophysical constraints. A high normalized moment of inertia (MoI) of 0.346 ± 0.014 , in combination with thermal and geochemical constraints, favors models with an Earth-like mantle density of $\sim 3300 \text{ kg/m}^3$, an inner core $\leq 1050 \text{ km}$ in radius, and a core silicon content of at least 6 wt%. In contrast, a lower value of $\text{MoI} = 0.333 \pm 0.005$ favors models with lower mantle densities of $\sim 3100 \text{ kg/m}^3$, an inner core radius in the range of 850–1,450 km, and a core silicon content less than 8 wt%. We also show that the formation of iron snow requires a sulfur concentration greater than $\sim 4 \text{ wt\%}$. However, the expected geochemistry of the core restricts the sulfur content to less than 2 wt%. This inconsistency suggests the absence of snow layers in Mercury's present-day core and that its dynamo is not driven by sulfur-induced iron crystallization.

Plain Language Summary Geophysical measurements that provide information on the distribution of mass inside a planet, or its Moment of Inertia (MoI), can be utilized to estimate Mercury's interior structure. We use interior structure models informed by two published MoI values to constrain Mercury's inner core size and test the iron snow hypothesis for dynamo generation, where convection is driven by iron precipitation within the outer core. Our results broadly show that lower MoI values favor models with moderate inner core sizes (850–1,450 km) and lower silicon concentrations (2–7 wt%), while higher MoI values favor models with potentially small inner cores (less than $\sim 1050 \text{ km}$) and higher silicon concentrations (at least 6 wt%). We also find a strong correlation of mantle density with MoI: higher MoI values yield Earth-like mantle densities, whereas lower MoI values imply lower densities. We find that iron snow forms only when core sulfur exceeds the amount suggested by geochemical data. This mismatch implies that Mercury's core likely lacks snow layers and that its dynamo has a different power source.

1. Introduction

Mercury is an ideal target for studying how rocky planets evolve. Its large core, which is partially liquid (Margot et al., 2007, 2012) and the seat of a weak magnetic field driven by dynamo action (Anderson et al., 2011), is unique among terrestrial planets. This provides a motivation to further understand Mercury's interior structure, which would allow us to further understand both how the planet evolved and how its magnetic field is driven within the core. In doing so, we may learn valuable insights on the evolution of other terrestrial planets. Without in situ measurements from a seismometer, we rely on measurements and modeling to infer Mercury's interior structure. Ground-based radar observations (Margot et al., 2007, 2012) and measurements by the MERcury Surface, Space, ENvironment, GEOchemistry, and Ranging (MESSENGER) satellite mission (Solomon et al., 2011) provide geodetic, geochemical, and magnetic constraints needed to model and constrain Mercury's interior. Upcoming measurements from the *BepiColombo* mission (Benkhoff et al., 2010) will provide further constraints.

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1.1. Core Structure

The structure of Mercury's core can be inferred through a number of geophysical and geodetic parameters. Measurements of the gravitational parameter $GM = 22,031.86 \times 10^9 \text{ m}^3/\text{s}^2$ (Genova et al., 2019; Konopliv et al., 2020; Verma & Margot, 2016), where G is the gravitational constant, imply that Mercury's mass is $M = 3.301 \times 10^{23} \text{ kg}$ which, together with its mean spherical radius $R = 2439.36 \text{ km}$ (Perry et al., 2015), yield a mean density of $\bar{\rho} = 5429.3 \text{ kg/m}^3$. In addition, a key geophysical constraint is the normalized polar moment of inertia $\tilde{C} = C/MR^2$, where C is the polar moment of inertia (MoI). $\tilde{C}$ gives a measure of how centrally concentrated the mass of the planet is. Observations of Mercury's obliquity θ (the angle between the spin axis and the normal to the orbital plane) under the assumption that it occupies a Cassini state provides an estimate of $\tilde{C}$ given by (Peale, 1976a; Peale et al., 2002; Zuber et al., 2007):

$$\tilde{C} = \frac{C}{MR^2} = \frac{n}{|\mu|} \frac{G_{210}J_2 + 2G_{201}C_{22}}{\sin I/\theta + \cos I}, \quad (1)$$

where n is the mean motion, μ is the rate of precession, I is the inclination of Mercury's orbit with respect to the Laplace plane, G_{210} and G_{201} are functions of the orbit eccentricity e (Baland et al., 2017; Yseboodt & Margot, 2006; Zuber et al., 2007), and J_2 and C_{22} are the unnormalized degree 2 coefficients of Mercury's gravity field.

A geodetic constraint used to infer the state of the core is the 88-day longitudinal libration amplitude ϕ_0 caused by the periodically reversing solar torque, given by (e.g., Zuber et al., 2007):

$$\phi_0 = \frac{3}{2} f_1 \frac{B - A}{C_m}, \quad (2)$$

where $f_1 = 1 - 11e^2 + \frac{959}{48}e^4$, $B > A$ are the two principal equatorial MoI, and C_m is the polar MoI of the solid part of Mercury. If the core is solid, the whole planet librates as a single body and $C_m = C$. If instead the core is partially fluid, it is principally the mantle that librates, so $C_m < C$, which leads to a larger ϕ_0 (Peale, 1976b). Margot et al. (2012) used ground-based radar to obtain measurements of the libration amplitude and obliquity of Mercury, finding $\phi_0 = 38.5 \pm 1.6 \text{ arcsec}$ and $\theta = 2.04 \pm 0.08 \text{ arcmin}$. Combined with the gravity field measurements of J_2 and C_{22} , these yield $\tilde{C} = 0.346 \pm 0.014$ and $C_m/C = 0.426 \pm 0.025$ (Margot et al., 2012), demonstrating that the core is at least partially fluid. After analyzing the 4 years of MESSENGER radio science measurements, Genova et al. (2019) found a lower obliquity of $\theta = 1.968 \pm 0.027 \text{ arcmin}$, which lowers $\tilde{C}$ to 0.333 ± 0.005 and raises C_m/C to 0.443 ± 0.007 .

Several other measurements of Mercury's obliquity have been reported (e.g., Bertone et al., 2021; Konopliv et al., 2020); see Table 1 of Goossens et al. (2022) for a compilation of results. The measured obliquities and determinations of the pole position (e.g., Bertone et al., 2021; Genova et al., 2019) are consistent with Mercury being in a Cassini state, and generally fall into two categories: obliquities close to 2.04 arcmin similar to that measured by Margot et al. (2012) or close to $\theta = 1.97 \text{ arcmin}$ as measured by Genova et al. (2019). The reason for this difference remains unknown. Measurements based on tracking surface features (e.g., Bertone et al., 2021; Margot et al., 2012) reflect the orientation of the spin axis of the solid outer shell (mantle and crust), while measurements based on the gravity field (e.g., Genova et al., 2019; Konopliv et al., 2020) reflect instead the tilt of the mean moment of inertia. The mantle, fluid core, and solid inner core (if present) could spin at different orientations (e.g., Dumberry, 2021; Peale et al., 2016), which could explain a part of the discrepancy. Nevertheless, the two obliquity estimates imply different MoI, which can be categorized as either a high value close to $\tilde{C} \sim 0.346$ or a low value close to $\tilde{C} \sim 0.333$.

Equation 2 is strictly valid only if the entire core is fluid. If a solid inner core is present, the prediction of ϕ_0 is altered by a factor of $(1 + \xi)$ (Dumberry & Rivoldini, 2015; Dumberry et al., 2013; Steinbrügge et al., 2021):

$$\phi_0 = \frac{3}{2} \frac{f_1}{(1 + \xi)} \frac{B - A}{C_m}. \quad (3)$$

The correction factor ξ represents the relative difference in the mantle libration amplitude, that is, predicted with and without an inner core, and it depends on the inner core size and the interior density structure of the whole planet (Dumberry & Rivoldini, 2015; Steinbrügge et al., 2021). The constraints on C_m/C given above for the two different estimates of $\tilde{C}$ neglect this correction factor. For large inner cores, ξ can be sufficiently large to affect the relationship between ϕ_0 and C_m (Van Hoolst et al., 2012), and it is better to use ϕ_0 as a constraint directly, rather than C_m/C inferred from Equation 2. The numerical value of ξ is a function of the interior density structure so it is not known a priori. However, it can be calculated for a given density model (Dumberry et al., 2013).

Models of the interior density structure of Mercury must match, along with $\bar{\rho}$, the constraints $\tilde{C}$ and ϕ_0 . In turn, these provide a relatively tight bound on the possible radius of the outer core. Although its exact value depends on the choice of $\tilde{C}$ (high or low value) and the choice of core composition among other factors, the outer core radius is approximately equal to 2,000 km (Dumberry & Rivoldini, 2015; Goossens et al., 2022; Hauck et al., 2013; Margot et al., 2018; Steinbrügge et al., 2018, 2021). The radius of the solid inner core, in contrast, remains poorly constrained, although the lower estimate of $\tilde{C}$ favors inner core sizes larger than 1,000 km (Genova et al., 2019; Goossens et al., 2022; Steinbrügge et al., 2021).

An additional constraint on Mercury's interior comes from the tidal Love number k_2 which quantifies how a planet deforms subject to tidal forces. It depends primarily on the rheology and thickness of the mantle but is also sensitive to the size of the liquid core. A high k_2 implies a large fluid core and a warm, weak mantle; conversely, a low k_2 implies a smaller core and a colder, stiffer mantle. The most recent estimates based on MESSENGER data are $k_2 = 0.569 \pm 0.025$ (Genova et al., 2019) and $k_2 = 0.53 \pm 0.03$ (Konopliv et al., 2020). These are higher than previous estimates (Mazarico et al., 2014; Verma & Margot, 2016), suggesting that the mantle may be warmer and weaker than previously believed (Padovan et al., 2014; Steinbrügge et al., 2021).

1.2. Core Composition

Given Mercury's large core, its density (and thus, its composition) plays a key role in the predictions of $\bar{\rho}$, $\tilde{C}$ and ϕ_0 built from interior models. Analyses of MESSENGER measurements suggest iron (Fe) and sulfur (S) contents of 1–4 wt% at the surface (Chabot et al., 2014; Evans et al., 2012; Nittler et al., 2011; Starr et al., 2012; Weider et al., 2012). These values support the idea that Mercury's core formed under highly reducing conditions (McCubbin et al., 2012; Pommier, 2025; Zolotov et al., 2013). Chabot et al. (2014) investigated different combinations of S and silicon (Si) in the Fe-S-Si system and placed constraints based on which ones were in equilibrium with silicate melts and consistent with surface S contents. They found combinations that are consistent with S contents at the surface, but not with Fe surface concentrations. These results suggest that Si is likely present in the core. Bounds on the expected Si and S content within the core can be set if we assume that a solid inner core has nucleated at the center of Mercury. For a Fe-Si alloy, an inner core can only form for Si weight fractions of 7–12 wt% (Edmund et al., 2022). For a Fe-S alloy, to ensure that the core-mantle boundary (CMB) temperature is within a reasonable range of 1850–2200 K, the presence of an inner core places an upper bound of S < 5 wt% (Rivoldini et al., 2009). As a more stringent upper bound, since Mercury's core is expected to have formed under highly reducing conditions (e.g., McCubbin et al., 2012; Pommier, 2025; Zolotov et al., 2013), we expect a Si-rich core with no more than 2 wt% S (Namur et al., 2016).

Recently, Steinbrügge et al. (2021) considered possible interior models of Mercury with end-member core compositions of pure Fe-S or pure Fe-Si. They investigated how the requirement of matching either the higher MoI value $\tilde{C} = 0.346 \pm 0.014$ from Margot et al. (2012) or the lower $\tilde{C} = 0.333 \pm 0.005$ from Genova et al. (2019) affected the resulting interior models. They found that matching the lower $\tilde{C}$ required a low mantle density (2900 – 3200 kg/m³). Other studies have reached the same conclusion (e.g., Goossens et al., 2022; Knibbe et al., 2021). These densities are at the low end of those compatible with mineralogical models (between 3000 – 3350 kg/m³ in Malavergne et al. (2010)), but could be explained by a sulfide-rich mantle (yielding average mantle densities between 3040 – 3100 kg/m³ (Lark et al., 2022; Steinbrügge et al., 2021)).

One limitation of the study by Steinbrügge et al. (2021) and of other similar studies (e.g., Genova et al., 2019; Goossens et al., 2022) is that only end-member core compositions of either Fe-S or Fe-Si were considered. As they noted, while the core might be Si-dominated, some amount of sulfur must be present, and this may help to

alleviate some of these problems. Our present study is motivated in part by the need to consider a more realistic core composition that includes both Si and S.

1.3. Core Dynamo

Mantle properties control the rate of heat flow out of the core, providing another constraint on core structure via the dynamo. Mercury's intrinsic magnetic field is anomalously weak with a surface intensity about 100 times weaker than the Earth's and has a topology characterized by an axisymmetric dipole with a significant northward offset (Anderson et al., 2011; Johnson et al., 2012). The heat flow at Mercury's CMB is expected to be sub-adiabatic (Davies et al., 2024; Grott et al., 2011; Hauck et al., 2004; Knibbe et al., 2025; Tosi et al., 2013), implying that the top of the core should be thermally stratified. This further implies that some form of compositional convection must occur in order to drive the dynamo (e.g., Dumberry & Rivoldini, 2015).

While several hypotheses have been put forward to power Mercury's dynamo (e.g., Kolhey et al., 2025; Soderlund et al., 2024; Tikoo & Evans, 2022), we focus here on scenarios associated with core crystallization (e.g., Breuer et al., 2015; Hauck et al., 2006). If Mercury's core is sufficiently sulfur-enriched, the inflections in the liquidus curve at Mercury's core pressure are such that iron-rich snow may form in a layer (or multiple layers) near the CMB (Chen et al., 2008). This heavy, sinking snow melts once underneath the snow-forming layer, and this dense Fe-rich melt drives convection, possibly leading to dynamo action (e.g., Dumberry & Rivoldini, 2015). In contrast, if the sulfur content is too low, then Earth-like inner core crystallization from the center outward is more likely. If Mercury's dynamo is driven by convection beneath a snow layer, their presence must be predicted by interior models. Alternatively, models lacking snow layers would suggest that dynamo action is unrelated to iron snow crystallization. Thus, geodetically and geophysically constrained interior models can shed light on Mercury's dynamo generation mechanism and vice versa.

In this study, we build upon the previous work of Dumberry and Rivoldini (2015) and Steinbrügge et al. (2021). In an attempt to address the challenges identified in the latter study, we build equations of state that incorporate the latest laboratory data for the Fe-S-Si system (Section 2). We investigate the possible Fe-S-Si core compositions and interior models that are compatible with the constraints on $\tilde{C}$ and ϕ_0 , separately for both the high and low estimates of $\tilde{C}$. Our first objective is to refine our understanding of how specific choices of $\tilde{C}$ affect interior models. In particular, we aim to understand how the choice of $\tilde{C}$ can further inform us on the size of the inner core, the mantle density, and the Si content of the core. A distinct advantage of our modeling strategy compared to other studies (e.g., Genova et al., 2019; Goossens et al., 2022) is an anchoring of the temperature at the ICB to the melting temperature of the core alloy, and tracking regions in the fluid core where the temperature falls below the melting point to identify where Fe-rich snow forms. Hence, we further investigate the core compositions that are compatible with the presence of snow layers, with an aim to determine the likelihood that Mercury's dynamo is driven by a crystallization regime that features iron snow.

2. Interior Models

Our method to build interior models of Mercury follows Dumberry and Rivoldini (2015) and is also described in the supplement of Steinbrügge et al. (2021). We assume a spherically symmetric planet with a silicate crust (of thickness h_{cr}), a mantle, a fluid outer core (CMB radius r_{CMB}), and a solid inner core (radius r_{ICB}). The density (ρ) is assumed uniform in both the crust and mantle, but it is radially variable within the inner core and fluid core and depends on composition, pressure, and temperature. The radial (r) variations in pressure (P) and gravitational acceleration (g) are governed by the condition of hydrostatic equilibrium and Poisson's equation, which are, respectively:

$$\frac{dP}{dr} = -\rho g, \quad (4)$$

$$\frac{dg}{dr} = 4\pi G\rho - \frac{2g}{r}. \quad (5)$$

Table 1
Input Parameters for Our Mercury Interior Models

Input	Definition	Value
R	Mercury Radius (Perry et al., 2015)	2439.36 km
ρ_{cr}	Crustal Density (Sori, 2018)	2974 kg/m ³
h_{cr}	Crustal Thickness (Sori, 2018)	26 km
GM	Gravitational Parameter (Genova et al., 2019)	$22031.86 \times 10^9 \text{ m}^3/\text{s}^2$
r_{ICB}	Inner Core Radius	0–2000 km
χ_{Si}	Core Silicon Weight Fraction	1–12 wt%
C/MR^2	Normalized MoI (Margot et al., 2012)	0.346 ± 0.014
	Normalized MoI (Genova et al., 2019)	0.333 ± 0.005
ϕ_0	Libration Amplitude (Margot et al., 2012)	$38.5 \pm 1.6 \text{ arcsec}$

The inner core of Mercury is likely in a conductive state, as is modeled in Knibbe et al. (2025), but for convenience we assume an adiabatic temperature profile. Radial variations in temperature (T) within the solid inner core and within the convecting regions of the fluid core are governed by its adiabatic gradient:

$$\frac{dT}{dr} = -\frac{\gamma}{K_s} \rho g T, \quad (6)$$

where γ is the Gruneisen parameter and K_s the adiabatic bulk modulus. In the outermost region of the fluid core, between a radius r_{ta} and the CMB, a sub-adiabatic temperature gradient is imposed, decreasing linearly from its adiabatic value at r_{ta} to a fraction ζ at the CMB, as given by

$$\frac{dT}{dr} = -\left(1 - (1 - \zeta) \frac{r - r_{ta}}{r_{CMB} - r_{ta}}\right) \frac{\gamma}{K_s} \rho g T. \quad (7)$$

The thickness of the thermally stratified layer and the heat flux at the CMB depends on the thermal history of Mercury (e.g., Davies et al., 2024; Knibbe et al., 2025; Knibbe & van Westrenen, 2018). Here, we set the base of the layer as the mid-depth of the fluid core ($r_{ta} = r_{ICB} + (r_{CMB} - r_{ICB})/2$) and the fraction of the heat flux at the CMB is set to $\zeta = 0.05$ as in Dumberry and Rivoldini (2015). Different choices of r_{ta} , ζ , as well as crustal depth h_{cr} , have a minimal effect on model solutions (Dumberry & Rivoldini, 2015; Steinbrügge et al., 2021).

In addition to Equations 4–7, equations of state (EoS) relating ρ , K_s , and γ to composition, P , and T are supplemented within the core; these are described in Dumberry and Rivoldini (2015). In all models, the ICB temperature is set equal to the liquidus (i.e., melting temperature) of the outer core to serve as an anchor point for the integration in radius of the temperature profile. This melting temperature depends on the composition, and we describe below how it is computed as a function of the weight fractions of sulfur (χ_S) and silicon (χ_{Si}).

For chosen values of h_{cr} , r_{ta} , and ζ , individual interior models are specified by two free parameters: the inner core radius and the weight fraction of silicon in the core. The weight fraction of sulfur is an output, controlled by the EoS and changes with radius in snow zones (see below). The radial profiles of P , g , T , ρ , and χ_S are constructed by integrating Equations 4–7 from the center to the surface (R), with the requirement of matching Mercury's mass M (or, equivalently, its mean density $\bar{\rho}$), the libration amplitude ϕ_0 (including the correction for the inner core using Equation 3), and specific values of $\tilde{C}$. The procedure is based on a shooting method, where initial guesses for the central T and P , R_{CMB} , mantle density, and S concentration at the ICB are iteratively adapted until the radial integration produces a model that matches M , ϕ_0 , $\tilde{C}$, as well as P matching the hydrostatic pressure at R_{CMB} and T matching the liquidus at the ICB.

The list of input parameters for our interior models, which include M , ϕ_0 , and $\tilde{C}$, is given in Table 1. Our adopted values for ρ_{cr} and h_{cr} are based on Sori (2018) although these are not well constrained (e.g., Beuthe et al., 2020). Different choices for ρ_{cr} and h_{cr} do not have a significant influence on our results, except for the resulting mantle

Table 2
Liquid Iron Chemical Potential Interaction Parameters

	$L_{i,1}/(\text{kJ})$	$L_{i,2}/(\text{kJ/K})$	$L_{i,3}/\text{kJ/GPa}$	$L_{i,4}/(\text{kJ/GPa}^2)$
$i = 1$	38.6794	-0.0171397	-1.71709	0.279949
$i = 2$	-3.73015	0.0204278	-2.93656	0.113838

density, which must adapt so as to yield the same MoI of the silicate shell (and thus, the same ϕ_o). As a metric, increasing (decreasing) h_{cr} to 50 km (10 km) leads to an increase (decrease) in mantle density of approximately 50 kg m^{-3} . Examples of their influences on the results are shown in Figure 11 of Dumberry and Rivoldini (2015) for a Fe-S core; results are similar for the Fe-S-Si core that we consider here.

The choice of $\tilde{C}$ is based on either the “high” or the “low” estimates, which we take here as those obtained, respectively, by Margot et al. (2012) and Genova et al. (2019):

$$\text{High : } \tilde{C} = 0.346 \pm 0.014 \quad (\text{Margot et al., 2012}), \quad (8a)$$

$$\text{Low : } \tilde{C} = 0.333 \pm 0.005 \quad (\text{Genova et al., 2019}). \quad (8b)$$

An essential ingredient of our method is the application of thermodynamic information of the core alloy to compute the liquidus and elastic properties as a function of depth and light element concentration. Here, we assume that the only light elements in the core are Si and S. The liquidus determines where crystallization occurs; it is tied to the radius of the inner core and controls the extent of snow regions in the fluid core.

The amount of S that partitions into solid Fe increases with pressure, but it is below 0.5 wt% at Mercury's core conditions (Li et al., 2001; Stewart et al., 2007) and therefore neglected. Unlike S, Si partitions almost equally between solid and liquid Fe. In the Fe-S-Si system, Si preferably partitions into solid Fe and the amount of Si in solid Fe increases with S (Tao & Fei, 2021). Although the difference can be as large as a few wt% for the maximal amount of Si considered in this study, we assume that Si partitions equally between solid Fe and liquid Fe-S.

The combined effect of S and Si on the melting temperature of Fe is not well known at Mercury's core conditions (Sakairi et al., 2017; Tao & Fei, 2021). For this reason, we approximate the melting temperature of Fe-S-Si by combining the effects that S and Si individually have on the melting temperature of Fe ($T_{m,Fe}$). The melting temperature is expressed as

$$T_{m,FeSi}(\chi_S, \chi_{Si}, P) = T_{m,Fe}(P) + \Delta T_S(\chi_S, P) + \Delta T_{Si}(\chi_{Si}, P), \quad (9)$$

where

$$\Delta T_S(\chi_S, P) = T_{m,FeS}(\chi_S, P) - T_{m,Fe}(P), \quad (10)$$

$$\Delta T_{Si}(\chi_{Si}, P) = T_{m,FeSi}(\chi_{Si}, P) - T_{m,Fe}(P), \quad (11)$$

and $T_{m,FeS}$ and $T_{m,FeSi}$ are the melting temperature of Fe-S and Fe-Si, respectively.

The melting temperature of Fe-S is computed from the thermodynamic model of Hillert and Staffansson (1975) that we have extended to high pressure. The interaction parameters that account for the non-ideal mixing of Fe and S and that are part of the chemical potential parameterization of liquid Fe write as

$$L_i(P, T) = L_{i,1} + L_{i,2}T + L_{i,3}P + L_{i,4}P^2, \quad (12)$$

where $i = 1, 2$. The interaction parameters that have been estimated by fitting the thermodynamic model to experimental melting data (Brett & Bell, 1969; Chen et al., 2008; Fei et al., 2000; Stewart et al., 2007; Walder & Pelton, 2005) are given in Table 2. Our Fe-S melting temperature parameterization is only valid for S concentrations below or equal to the eutectic.

We compute the Fe-S melting temperature through Gibbs energy minimization. If the very small dissolution of S in fcc Fe is neglected and the amount of S is below or equal to the eutectic, the melting temperature (e.g., Poirier, 2000) is the temperature at which the chemical potentials of l-Fe in l-Fe-S and pure fcc Fe are equal at a fixed pressure and composition. We use the expression of the composition-dependent chemical potential of l-Fe from

Hillert and Staffansson (1975) and the chemical potentials of pure l-Fe and fcc Fe from Komabayashi (2014). From the chemical potentials and interaction parameters (Equation 12 and Table 2) the Fe-S melting temperature can then be calculated as a function of S and pressure.

The melting temperature for Fe-Si is based on the results of Edmund et al. (2022). In our parameterization, $T_{m,FeSi}$ decreases linearly with χ_{Si} from $T_{m,Fe}$ to the eutectic temperature of Fe-Si ($T_{e,FeSi}$). Within the pressure range of the core, the eutectic concentration $\chi_{e,FeSi}$ is almost pressure independent and set to 12 wt% (Edmund et al., 2022). We also neglect the small temperature difference between solidus and liquidus. We write the melting temperature of Fe-Si as

$$T_{m,FeSi}(\chi_{Si}, P) = T_{m,Fe}(P) + (T_{e,FeSi}(P) - T_{m,Fe}(P)) \frac{\chi_{Si}}{\chi_{e,FeSi}}. \quad (13)$$

Finally, for the parametrization of $T_{m,Fe}$, we follow Anzellini et al. (2013) and use

$$T_{m,Fe}(P) = a_1(P_0 - P)^{a_2}, \quad (14)$$

where $a_1 = 495.5 \text{ K GPa}^{-a_2}$, $a_2 = 0.42$, and $P_0 = 22.2 \text{ GPa}$.

As part of the radial integration of the temperature profile, when the temperature at a given radius in the fluid core drops below the liquidus T_m , solid Fe-Si compounds crystallize to form iron-rich snow and increase sulfur content locally. The sulfur concentration $\chi_S(r)$ is then updated such that $T(r) = T_m(\chi_S(r), \chi_{Si}, P(r))$. This updated χ_S is used to further update the temperature and liquidus at a larger radius along the integration path. If at some further radius $T > T_m$, this marks the top boundary of the snow region, and the sulfur concentration remains fixed above this point.

3. Results

The modeling strategy described above allows us to study a range of possible interior models spanning different values of inner core radius (r_{ICB} , varied in increments of 50 km) and Si concentration (χ_{Si} , varied in increments of 1 wt%) while matching specific choices of $\tilde{C}$. For each combination of r_{ICB} and χ_{Si} , we randomly draw 1024 values of $\tilde{C}$ from a normal distribution based on either the high or low estimate (Equations 8a or 8b, respectively), and for each of these individual $\tilde{C}$ values we attempt to build an interior model. Sampling $\tilde{C}$ from a normal distribution provides a good sampling of the parameter space while tying the resulting interior models to geophysical observations. For some combinations of r_{ICB} , χ_{Si} and $\tilde{C}$, it is not possible to find a model, that is, also compatible with the libration amplitude ϕ_0 and mass M ; these failed models are discarded. For each combination r_{ICB} and χ_{Si} , out of the 1024 drawn values of $\tilde{C}$, we find up to a few hundred successful interior models that can match ϕ_0 and M . This gives a probability distribution of interior structure models as a function of r_{ICB} and χ_{Si} for each of the high and low choices of $\tilde{C}$ (see top row of Figure S5 in Supporting Information S1). Overall, for each of the high and low $\tilde{C}$, we find approximately 10^5 successful models (the posterior distributions of $\tilde{C}$ values are shown in top row of Figure S6 in Supporting Information S1). We deem this set of models to be sufficient for our results to be statistically reliable. From this set of models, we investigate those that also match a series of additional thermal, compositional, and iron-snow formation constraints.

This strategy for sampling the interior model parameter space differs from that adopted in Genova et al. (2019) and Goossens et al. (2022). Those studies use a Markov Chain Monte Carlo (MCMC) framework, with target normal distributions of $\tilde{C}$ (low or high) guiding the probability of the models. Our approach is different because our interior models are constructed to match specific values of $\tilde{C}$. In this sense, $\tilde{C}$ is an input to our models, rather than an inferred output. We draw samples of $\tilde{C}$ from the low and high distributions separately, and the resulting distribution of $\tilde{C}$ among the successful models indicates which MoI values are favored by our interior models.

3.1. Thermal Constraints

We restrict the number of successful models on the basis of their CMB temperatures. Since present-day magmatic activity is unlikely and mantle melting is expected above $\sim 2000 \text{ K}$ (Namur et al., 2016), this sets an upper limit on

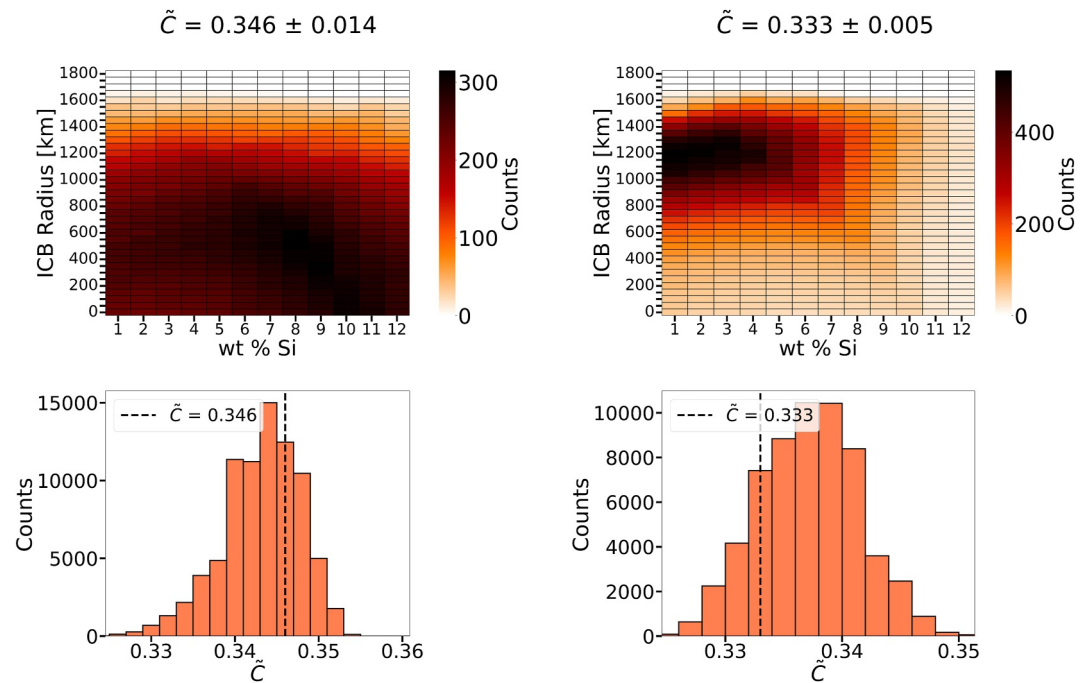


Figure 1. Interior models with T_{CMB} in the range 1700–2100 K. Top row: probability distributions of r_{ICB} and χ_{Si} from interior models sampled from the high (left) and low (right) MoI constraints. Bottom row: Probability distributions of $\tilde{C}$, with a bin size of 0.002, from interior models sampled from the high (left) and low (right) MoI constraints.

T_{CMB} . Conversely, widespread volcanism in Mercury's past (Denevi et al., 2013; Head et al., 2011; Marchi et al., 2013; Thomas et al., 2014) implies that mantle temperatures previously exceeded 2000 K. Assuming a global cooling by $\lesssim 200$ K over the past 4.5 Gyr (Byrne et al., 2014; Edmund et al., 2022; Grott et al., 2011; Hauck et al., 2004) sets a lower limit of $T_{CMB} \sim 1800$ K. Allowing for a slightly wider range of T_{CMB} , our thermal criteria for a successful model is set to $1700 \text{ K} \leq T_{CMB} \leq 2100 \text{ K}$.

Figure 1 (top row) shows the probability distribution of r_{ICB} and χ_{Si} for interior models that are compatible with our specified range of T_{CMB} , for each of the high and low $\tilde{C}$ scenarios. Possible models exhibit a wide range of inner core sizes, from no inner core up to $r_{ICB} = 1650$ km, and also a wide range of Si concentrations up to 12 wt% (the maximum value considered). The most probable (i.e., higher count) set of r_{ICB} and χ_{Si} depends on the choice of $\tilde{C}$, and the criteria for the most probable models are defined in the supplementary text, including Figures S9 and S10 in Supporting Information S1. The high $\tilde{C}$ values favor models with an inner core smaller than 1000 km while not discriminating strongly on the Si content; the low $\tilde{C}$ values instead favor models with inner core radii between 950 and 1,400 km and Si concentrations ≤ 5 wt%. These results are generally consistent with previous studies that assumed a core composition of either Fe-Si (e.g., Goossens et al., 2022; Steinbrügge et al., 2021) or Fe-Si-C (Knibbe et al., 2021); taking into account a Fe-S-Si core alloy does not lead to a drastic change in the way interior models are tied to $\tilde{C}$.

Figure 1 (bottom row) shows the probability distribution of $\tilde{C}$ for all successful models, encompassing the full range of r_{ICB} and χ_{Si} . The number of successful models that match the constraint T_{CMB} drawn from the high MoI scenario is maximum at $\tilde{C} \approx 0.343$ – 0.345 , and generally high in the range of 0.339 – 0.349 , encompassing the central value of 0.346 of its prior distribution. Likewise, the number of successful models drawn from the low $\tilde{C}$ scenario is maximum at $\tilde{C} \approx 0.336$ – 0.34 , high in the range 0.332 – 0.342 . These posterior-like distributions give a measure of the $\tilde{C}$ value, that is, preferred by our interior models. Broadly, they indicate that models that meet the T_{CMB} constraint favor a MoI closer to $\tilde{C} \approx 0.34$ – 0.342 , in-between the low and high geodetic estimates of Genova et al. (2019) and Margot et al. (2012). Probability distribution maps and MoI histograms that cover additional samples from our Monte Carlo simulations can be found in Figures S5 and S6 of the Supporting Information S1.

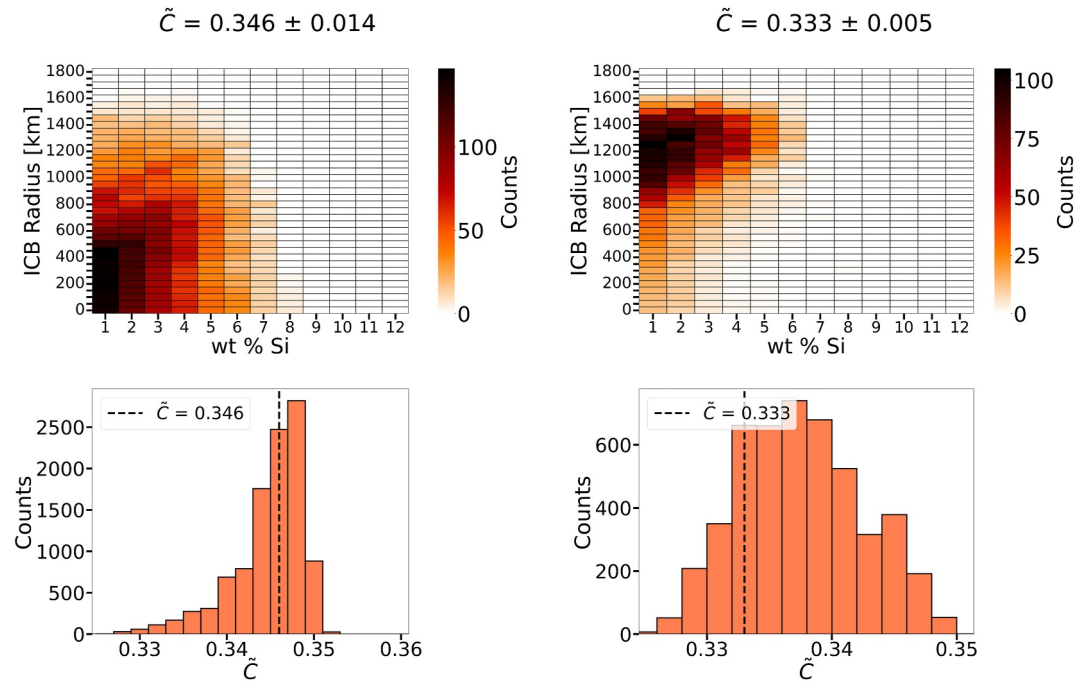


Figure 2. Interior models with T_{CMB} in the range 1700–2100 K and which feature an iron snow layer that does not extend to the ICB. Top row: probability distributions of r_{ICB} and χ_{Si} from interior models sampled from the high (left) and low (right) MoI constraints. Bottom row: Probability distributions of $\tilde{C}$, with a bin size of 0.002, from interior models sampled from the high (left) and low (right) MoI constraints.

3.2. Iron Snow Constraint

As an additional constraint, we further restrict the number of successful models to those that feature at least one snow layer that does not extend to the ICB. Such models would then also be compatible, at least in principle, with a dynamo mechanism associated with iron snow crystallization. Figure 2 shows the probability distribution of models that meet this criterion in addition to the constraint on T_{CMB} . The number of successful models is significantly reduced. The high $\tilde{C}$ values now favor models with an inner core smaller than 450 km (compared with <1000 km for the thermal constraint alone), while the range expands to 950–1,500 km for low $\tilde{C}$ values. Each choice of $\tilde{C}$ favors models with a Si concentration of ≤ 5 wt% and ≤ 4 wt% respectively.

Iron snow formation depends sensitively on the concentration of sulfur. Since S is restricted to the outer core, the bulk S weight fraction, averaged over the whole of the core, is given by

$$\chi_{S,bulk} = \frac{\int_{r_{ICB}}^{r_{CMB}} \chi_S(r) \rho(r) r^2 dr}{\int_0^{r_{CMB}} \rho(r) r^2 dr}. \quad (15)$$

For each combination of r_{ICB} and χ_{Si} , and for successful models that meet both T_{CMB} and snow layer constraints, the prior distributions of $\tilde{C}$ yield corresponding distributions of $\chi_{S,bulk}$.

Figure 3 shows the mean $\chi_{S,bulk}$ of this distribution (top row) and its coefficient of variation (CV, bottom row), defined as the ratio of the standard deviation to the mean. The CV provides a normalized metric for the dispersion around the mean of $\chi_{S,bulk}$ given that the samples for each combination of r_{ICB} and χ_{Si} vary in size. A CV of 0.1 indicates a standard deviation equal to 10% of the mean value. Thus, the CV values of ≈ 0.1 or lower observed for many of the $\chi_{S,bulk}$ distributions imply that the variations of $\chi_{S,bulk}$ with respect to mean values is typically less than 1 wt% S. The mean $\chi_{S,bulk}$ in the top row provides then a representative measure of the bulk S content within the core for each combination of r_{ICB} and χ_{Si} . The mean $\chi_{S,bulk}$ ranges between 1.9 and 7.8 wt%, although the vast majority of models have $\chi_{S,bulk} \gtrsim 4$ wt%. The lowest sulfur concentrations correspond to models with the largest

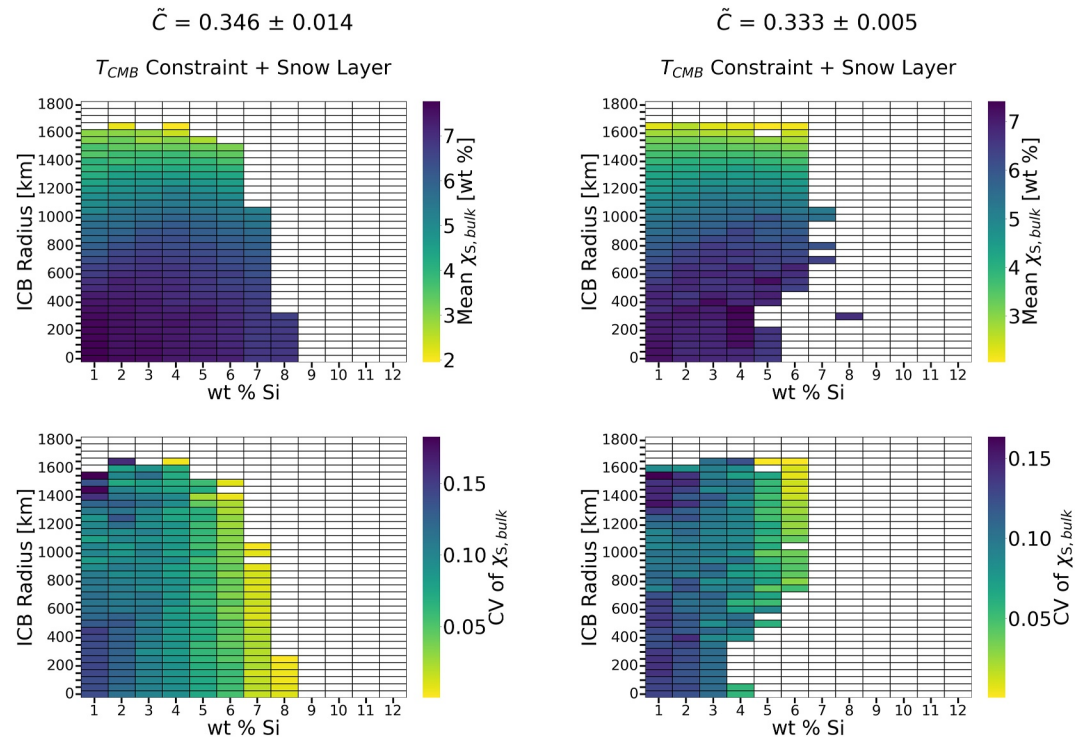


Figure 3. The mean values (top) and coefficients of variation (CV, bottom) of the bulk weight fraction of S in the core from models selected from the high (left) and low (right) MoI constraints with a T_{CMB} in the range 1700–2100 K and featuring an iron snow layer that does not extend to the ICB. Cases in which the mean $\chi_{S,bulk}$ is not accompanied by a corresponding CV value indicate that the sample size is one.

inner cores for each $\tilde{C}$ distribution. These results indicate that models with realistic CMB temperatures and snow layer geometries consistent with dynamo generation have sulfur contents larger a few wt%. Additional samples on $\chi_{S,bulk}$ can be found in Figures S7 and S8 of the Supporting Information S1.

Geochemical constraints suggest that the bulk S fraction in the core of Mercury is smaller than 2 wt% (Namur et al., 2016). Of all our models with a snow layer that meet the constraint on T_{CMB} , only a few also match $\chi_{S,bulk} < 2$ wt%: 3 models for the high MoI and 3 models for the low MoI. If indeed $\chi_{S,bulk}$ is smaller than 2 wt% in Mercury's core, by inference, it is unlikely that the dynamo is driven by iron snow.

3.3. Core Sulfur Concentration Constraints

Eliminating the requirement for iron snow formation, Figure 4 shows the probability distribution of r_{ICB} and χ_{Si} for models with $\chi_{S,bulk} < 2$ wt% and T_{CMB} in the range 1700–2100 K. Similar to Figure 1, the high MoI favors models that have an inner core radius ≤ 1050 km. In contrast, the added constraint on $\chi_{S,bulk}$ leads to a preference for relatively large Si concentrations of ≥ 6 wt%. The low MoI instead favors models that have an inner core radius in the range 850–1450 km and comparatively lower Si concentrations in the range of 2–7 wt%.

Combining all of the successful models shown in Figure 4 (both panels), Figure 5 shows how inner core radius (r_{ICB} , top left), core silicon content (χ_{Si} , top right), and the mean mantle density ($\bar{\rho}_m$, bottom left) depend on the MoI. While large inner cores are generally associated with lower $\tilde{C}$ values, a wide range of r_{ICB} remains permissible for any specific $\tilde{C}$, including the absence of an inner core. Hence, tight constraints on $\tilde{C}$ would narrow the possible range of r_{ICB} , but is unlikely to provide a definitive value. Core Si concentration is more linearly correlated with the MoI, with a larger $\tilde{C}$ permitting a larger χ_{Si} . We also observe a direct correlation between mantle density and MoI, where a higher $\tilde{C}$ corresponds to a higher $\bar{\rho}_m$. Here, the range of possible $\bar{\rho}_m$ values for a given $\tilde{C}$ is significantly narrower. For example, models with $\tilde{C} \approx 0.346$ have $\bar{\rho}_m$ between 3300 and 3350 kg/m³ while models with $\tilde{C} \approx 0.333$ have $\bar{\rho}_m$ between 3000 and 3100 kg/m³. These results are consistent with those

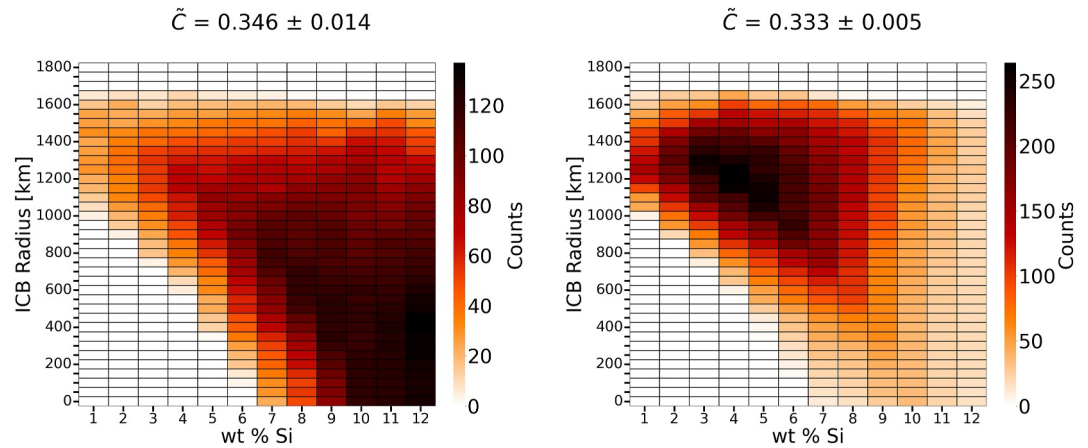


Figure 4. Interior models with T_{CMB} in the range 1700–2100 K and $\chi_{S,bulk} < 2$ wt%. Probability distributions of r_{ICB} and χ_{Si} sampled from the high (left) and low (right) MoI constraints.

obtained in other studies (Goossens et al., 2022; Knibbe et al., 2021; Lark et al., 2022; Steinbrügge et al., 2021). Figure 5 further highlights that a precise determination of $\tilde{C}$ provides a relatively tight constraint on mean mantle density as has been demonstrated for the Moon (Matsuyama et al., 2016). The bottom right panel of Figure 5 further shows that low $\tilde{C}$ and $\bar{\rho}_m$ values are consistent with larger inner cores. In contrast, larger $\tilde{C}$ and $\bar{\rho}_m$ values may have a wide range of possible inner core sizes.

4. Discussion and Conclusions

We have developed interior structure models of Mercury to evaluate which best fit the moments of inertia inferred from two separate studies: Margot et al. (2012) and Genova et al. (2019). Table 3 summarizes the most probable

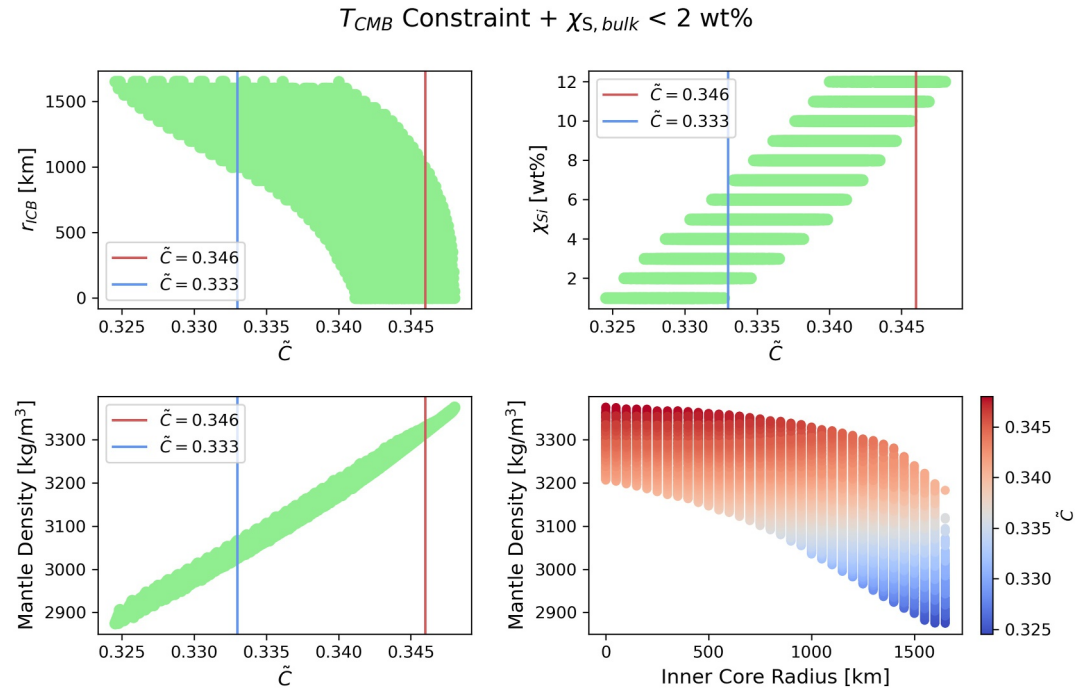


Figure 5. Inner core radius (top left), core Si concentration (top right), and average mantle density (bottom left) as a function of $\tilde{C}$. Bottom right: mean mantle density as a function of inner core radius, color contoured by $\tilde{C}$. Same data as shown in Figure 4, including both the high and low MoI distributions; thus, each dot represents an interior model with a T_{CMB} in the range 1700–2100 K and $\chi_{S,bulk} < 2$ wt%.

Table 3

Summary of Most Probable Inner Core Radii and Silicon Contents for Internal Structure Models Subject to the Thermal Constraint of $1700\text{ K} \leq T_{\text{CMB}} \leq 2100\text{ K}$ (See Top Row of Figure 1), the Thermal Constraint Plus the Required Existence of a Snow Layer That Does Not Extend to the Inner Core (See Top Row of Figure 2), and the Thermal Constraints in Addition to the Requirement for Less Than 2 wt% Bulk Sulfur Content in the Core (See Figure 4)

Constraint	r_{ICB} (km)		χ_{Si} (wt%)	
	High MoI	Low MoI	High MoI	Low MoI
T_{CMB}	≤ 1000	950–1400	1–12	≤ 5
T_{CMB} + Snow layer	≤ 450	950–1500	≤ 5	≤ 4
T_{CMB} + Sulfur content	≤ 1050	850–1450	≥ 6	2–7

inner core radii and silicon contents from these internal structure models subject to different constraints. In all scenarios, we restricted the models to have a CMB temperature compatible with past widespread mantle melting yet no present-day volcanism.

Motivated by the hypothesis that iron snow may drive Mercury's dynamo, we further applied the constraint that a snow layer not extending to the inner core must be present. Critically, our results show that iron snow formation typically requires a bulk S concentration larger than $\sim 4\text{ wt\%}$, well above geochemical expectations (Namur et al., 2016). This disagreement suggests that models with iron snow, regardless of the value of $\tilde{C}$, are difficult to reconcile with Mercury's likely composition and that the dynamo requires an alternate driving mechanism.

If we require the models to also have a bulk S fraction in the core smaller than 2 wt%, the two different constraints on $\tilde{C}$ lead to vastly different models of Mercury's interior. The high MoI constraint ($\tilde{C} \sim 0.346$) of Margot

et al. (2012) favors models that have an inner core radius smaller than 1050 km, a relatively large Si concentration in the core of at least 6 wt%, and a mean mantle density above 3300 kg/m^3 . The low MoI constraint ($\tilde{C} \sim 0.333$) of Genova et al. (2019) instead favors models that have an inner core radius exceeding 850 km, a lower Si concentration of 2–7 wt%, and a lower mantle density of $3000\text{--}3100\text{ kg/m}^3$. These results are broadly similar with those obtained on the basis of pure Fe-Si core alloy compositions (Goossens et al., 2022; Steinbrügge et al., 2021).

Beyond the consideration of an updated iron-sulfur-silicon core alloy composition, several other features of our interior models differ compared to those of similar recent studies (e.g., Genova et al., 2019; Goossens et al., 2022). Among these, notable distinctions include explicitly accounting for the inner core's influence on libration amplitude and incorporating a thermally stratified layer at the top of the core. These modeling differences do not cause major changes in the resulting interior models. For example, altering the stratification parameters affects the results by only a few percent (see for instance Figure 12 of Dumberry et al., 2013). Likewise, the inner core only contributes to a change smaller than 5% in the libration amplitude for models with a Fe-S core (see Figure 7 of Dumberry & Rivoldini, 2015), and the effect is weaker for a Fe-S-Si core since the density contrast at the ICB is reduced. Nevertheless, including their influence makes our models more realistic. Likewise, our modeling strategy includes linking the core temperature to the melting temperature of the core alloy at the ICB; this avoids the possible inconsistency of a temperature above the melting point within the inner core, or below it within the fluid core.

Additionally, while we draw samples of $\tilde{C}$ based on each of the high and low distributions, we do not guide the probability of our interior models based on matching these distributions. Instead, we keep a tally of the successful models and the distribution of their $\tilde{C}$ values gives an indication of the MoI, that is, favored by our interior models. We find that our models prefer a MoI which is closer to ~ 0.34 , approximately in between the low and the high estimates reported by Genova et al. (2019) and Margot et al. (2012), respectively.

Although the specific details between our individual models differ than those of Goossens et al. (2022), our results are in broad agreement, specifically in the way $\tilde{C}$ is tied to inner core size, outer core radius, CMB temperature, and mean mantle density. Hence, despite using different modeling strategies, a consistent picture of the interior structure of Mercury is emerging, albeit one that sensitively depends on $\tilde{C}$.

Our findings and conclusions are directly influenced by the liquidus parameterization of the core. This parameterization not only determines the inner core radius but also the occurrence and depth of the snow zones in the outer core. The experimentally determined melting data of Fe-Si and Fe-S-Si at Mercury core conditions is still rather limited and exhibits significant uncertainties. Our model of the liquidus aims to capture the available experimental data through a simple parameterization. Further experimental data is required, and substantial effort is necessary to construct a thermodynamic model capable of describing the complexities of the Fe-S-Si phase diagram. Any improvements will directly reflect on the occurrence of iron-rich snow and the core structure. Xu et al. (2021) show how the crystallization regimes of small planetary bodies may be affected by equations of state and Fe-S melting curves. They find that bottom-up crystallization regimes are more likely (as opposed to top-down regimes such as iron snow) for S-poor cores. Although their results only apply for pressures up to ~ 10

GPa, these are relevant for the upper core of Mercury. This further confirms that the occurrence of iron snow is strongly dependent on χ_S , and the likelihood of iron snow driving Mercury's dynamo primarily has to do with how χ_S compares to compositional constraints (e.g., Namur et al., 2016). Our results emphasize that, based on the current understanding of thermodynamic properties of iron alloys, iron-rich snow does not occur in a Fe-Si core at Mercury conditions, in line with the findings of Davies et al. (2024).

Goossens et al. (2022) showed that the high estimates of k_2 recently obtained by Genova et al. (2019) and Konopliv et al. (2020) tend to favor models that have a low $\tilde{C}$ compatible with a mean value near 0.333. This provides support for the low MoI of $\tilde{C} = 0.333 \pm 0.005$ derived by Genova et al. (2019). However, these models tend to have weak viscosities ($\leq 10^{16}$ Pa s) in their lowermost mantle near the CMB, as Steinbrügge et al. (2021) had found. Such a low viscosity presents its own challenges, as it should generate significant tidal dissipation and, consequently, should lead to an offset of the obliquity from an exact Cassini state larger than allowed by observations (Baland et al., 2017; MacPherson & Dumberry, 2022). As both Goossens et al. (2022) and Steinbrügge et al. (2021) point out, a possible solution to this problem is if the mantle is convecting (e.g., Davies et al., 2024) rather than purely conducting (e.g., Jain & Solomatov, 2024), as the more uniform temperature profile throughout the mantle implies a comparatively colder lowermost mantle and therefore a higher viscosity. Nevertheless, this serves to illustrate that there remains a number of question marks about Mercury's interior structure.

The joint European Space Agency and Japan Aerospace Exploration Agency *BepiColombo* mission, scheduled for orbital insertion around Mercury in 2026, is expected to provide an updated set of geodetic measurements and improve constraints on $\tilde{C}$. As our results show, both a more accurate and a more precise measure of $\tilde{C}$ are required to narrow the set of possible interior models of Mercury. Furthermore, h_2 measurements by the *BepiColombo* Laser Altimeter (BELA) will also be helpful in determining the size of Mercury's inner core when combined with k_2 measurements (Steinbrügge et al., 2018) and magnetic field measurements will enable better ties between internal structure with mechanisms of dynamo generation (Heyner et al., 2021). Additionally, measurements of the k_2 phase lag will improve our understanding of Mercury's mantle rheology (Genova et al., 2021). These measurements should be complimented by laboratory and theoretical studies on the behavior of iron alloys at Mercury's core conditions to further improve interior structure models (e.g., Genova et al., 2021).

Conflict of Interest

The authors declare no conflicts of interest relevant to this study.

Availability Statement

The software to model Mercury's interior is publicly available on GitHub repository <https://github.com/dunyuliu/PIE.git>. The repository is also attached as a zip file under <https://zenodo.org/records/16929504> (Dunnigan et al., 2025a). The simulation results are archived on <https://zenodo.org/records/16459292> (Dunnigan et al., 2025b).

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