

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

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1. Model results for the central $\tilde{C}$ values

In this work, we construct a suite of interior models that, for given choices of inner-core boundary radius (r_{ICB}) and silicon concentration (χ_{Si}), match values of either the high or the low MoI ($\tilde{C}$) constraints given in Eqs. (8a) and (8b) of the main text. Figure S1 shows how the core-mantle boundary (CMB) temperature (T_{CMB}), mean mantle density ($\bar{\rho}_m$), and bulk sulfur concentration averaged over the whole of the core ($\chi_{S,bulk}$) change as a function of r_{ICB} and χ_{Si} , for specific choices of $\tilde{C}$, namely, the central values of the two distributions of $\tilde{C}$, 0.346 and 0.333.

Let us highlight a few salient properties of the interior models shown in Figure S1. For a given χ_{Si} , in order to conserve mass, a larger inner core size is accompanied by an increase in $\chi_{S,bulk}$ and an increase in $\bar{\rho}_m$ (the latter results as a consequence of a larger CMB radius). In general, a larger χ_{Si} allows for larger possible inner core sizes. At a given χ_{Si} , the models which have an inner core size close to their maximum values have a significantly higher $\chi_{S,bulk}$ and higher $\bar{\rho}_m$ compared to models with small inner core sizes.

The trends for T_{CMB} reflect the temperature profile inside the core. For a given χ_{Si} , a larger inner core size implies a lower T_{CMB} . The reason for this is tied to the temperature at the ICB which, in our models, is set to the melting temperature of the Fe-S-Si alloy. Since a greater sulfur concentration (for models with a larger inner core size) implies a lower melting temperature, the whole temperature profile in the outer core is lowered, reducing T_{CMB} .

The choice of MoI significantly affects not only the model attributes but also the range of r_{ICB} and χ_{Si} for which viable models exist, primarily due to the internal mass distribution required by $\tilde{C}$. For a given χ_{Si} , the low MoI allows for larger possible ICB radii. For the

low MoI, no models are possible for $\chi_{\text{Si}} > 6$ wt %, and for χ_{Si} between 4 and 6 wt %, only models with a relatively large inner core (> 800 km) are possible. For choices of r_{ICB} and χ_{Si} where viable models exist for both high and low MoI values, the low MoI models have a lower $\chi_{\text{S,bulk}}$, a lower $\bar{\rho}_m$, and a higher T_{CMB} .

Complementing Figure S1, Figure S2 shows how the bulk density of the whole core ($\bar{\rho}_c$) and gravitational acceleration at the CMB (g_c) change as a function of r_{ICB} and χ_{Si} . These are given by

$$\bar{\rho}_c = \frac{M_c}{(4/3)\pi r_{\text{CMB}}^3}, \quad g_c = \frac{GM_c}{r_{\text{CMB}}^2}, \quad (1)$$

where M_c is the mass of the whole core. For the mean high MoI, the averages over all r_{ICB} and χ_{Si} values are $\bar{\rho}_c = 7007.06$ kg/m³ and $g_{\text{CMB}} = 3.96$ m/s². For the mean low MoI, the averages are $\bar{\rho}_c = 7588.17$ kg/m³ and $g_{\text{CMB}} = 4.17$ m/s². The higher core mass associated with the lower MoI illustrates the greater concentration of mass toward the centre; this is part of the reason why models that satisfy the low MoI also have a lower $\bar{\rho}_m$.

An additional model feature that we show in Figure S1 is the presence of iron snow zones in the outer core. These are regions of compositional stratification where the core temperature is equal to the melting temperature (e.g., Hauck et al., 2006; Dumberry & Rivoldini, 2015). Iron snow is a much more conspicuous feature of models that match the high MoI. Here, snow zones are present at small χ_{Si} for nearly all r_{ICB} , and restricted to models with relatively high ICB radii when $\chi_{\text{Si}} > 4$ wt %. In contrast, for the low MoI, snow zones are only possible in a narrow ICB radii band close to its maximal possible value ($1300 \text{ km} \leq r_{\text{ICB}} \leq 1500 \text{ km}$) and only for $\chi_{\text{Si}} < 5$ wt %.

Different iron snow zone regimes are possible (e.g., Dumberry & Rivoldini, 2015; Breuer et al., 2015). We use the terminology “layers” to refer to models that feature a single or multiple snow zones, and where the lower radius of the lower snow zone is above the ICB. When the lower snow zone extends down to the ICB, we use the terminology “deep snow” when no other snow layers are present above it and “deep snow + layers” when a snow layer is also present at a shallower depth. Figure S3 shows examples of these three regimes from our interior models. Of the three snow regimes, the “layers” and “deep snow + layers” regimes allow for snow-driven convective flows.

Figure S4 indicates which regimes the snow zone-bearing models from Figure S1 fall into. For the high MoI models, snow can develop even in the absence of an inner core for sufficiently low silicon contents and takes the form of deep snow with (1 wt% Si) and without (2 wt% Si) layers. For progressively larger inner core sizes for a fixed silicon concentration, the snow regime changes from “deep snow + layers” transitions to “layers” as the inner core grows to encompass the (former) snow region, to “deep snow” as the base of the snow layer extends deeper until it reaches the inner core boundary. This evolution can be seen in Figure S3. For the low MoI models, only six viable r_{icb} - χ_{Si} combinations develop snow and, of these, two are in the deep snow regime.

2. Additional model samples from Monte Carlo simulations

Figures S5, S6, S7, and S8 show the probability distributions, MoI histograms, and sulfur concentration statistics for more discrete samplings of the Monte Carlo simulations: all successful models, models with $1700 \text{ K} \leq T_{CMB} \leq 2100 \text{ K}$, models with a snow layer, and models that have both $1700 \text{ K} \leq T_{CMB} \leq 2100 \text{ K}$ and a snow layer.

3. Defining the most probable interior models

In this section, we define a threshold for determining the most likely values of r_{ICB} and χ_{Si} , based on the distributions of successful models presented in Figures 1 (subject to thermal constraints), 2 (subject to thermal and snow constraints), and 4 (subject to thermal and sulfur constraints) of the main text. Figures S9 and S10 recast these distributions as fractions of their respective maximum counts for the high and low MoI constraints, respectively. Combinations of r_{ICB} and χ_{Si} are considered most probable if their normalized counts are greater than or equal to 0.7.

References

- Breuer, D., Rückriemen, T., & Spohn, T. (2015). Iron snow, crystal floats, and inner-core growth: modes of core solidification and implications for dynamos in terrestrial planets and moons. *Progress in Earth and Planetary Science*, 2, 39. doi: 10.1186/s40645-015-0069-y
- Dumberry, M., & Rivoldini, A. (2015). Mercury's inner core size and core-crystallization regime. *Icarus*, 248, 254 - 268.
- Hauck, S. A., Aurnou, J. M., & Dombard, A. J. (2006). Sulfur's impact on core evolution and magnetic field generation on ganymede. *Journal of Geophysical Research: Planets*, 111(E9).

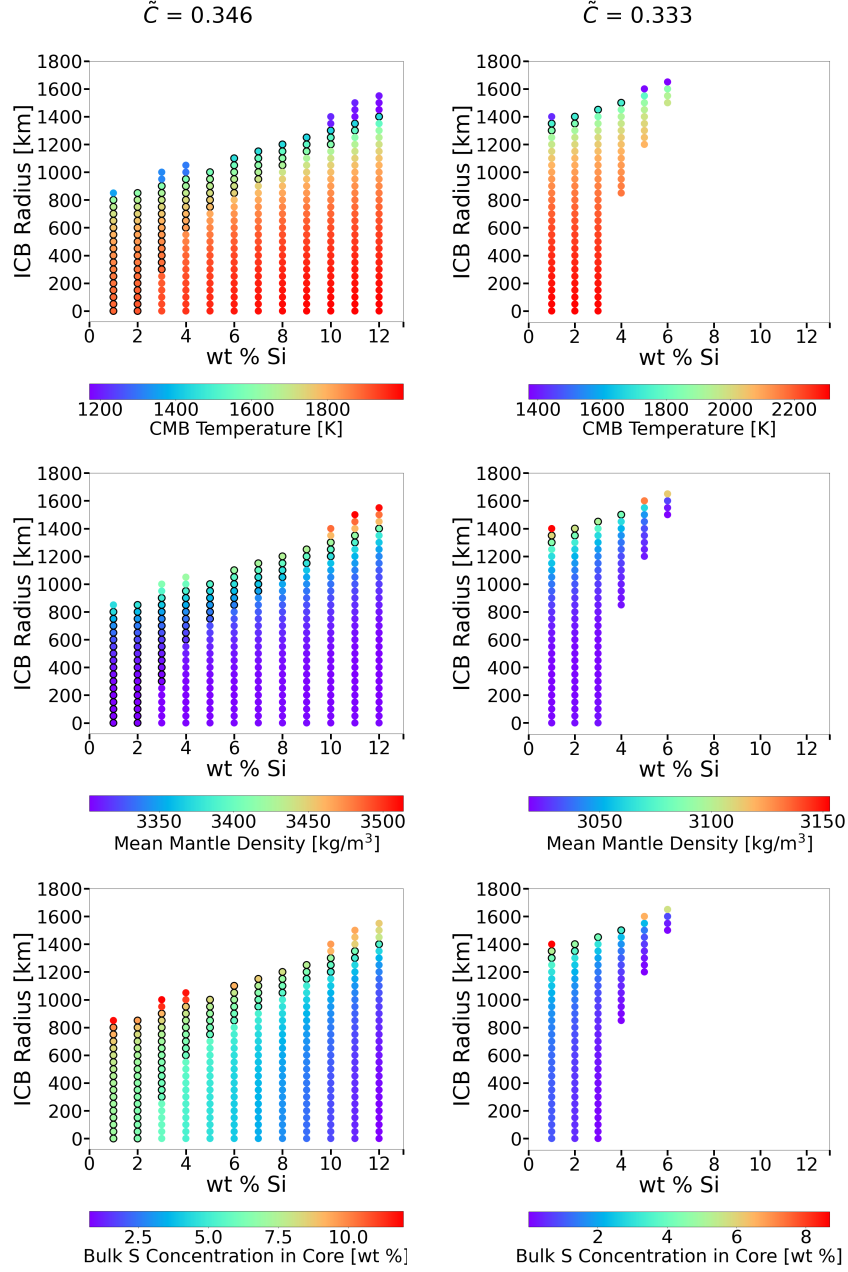


Figure S1. Core and mantle properties as a function of r_{ICB} and χ_{Si} for the mean high (left) and low (right) MoI constraints. Top: temperature at the core-mantle boundary, T_{CMB} . Middle: mean mantle density, $\bar{\rho}_m$. Bottom: bulk sulfur concentration in the core, $\chi_{S,bulk}$. Symbols with black outlines identify models that feature iron snow. Each color symbol corresponds to a singular interior model; absence of a symbol indicates that it is not possible to match the combination of $\tilde{C}$, mass M , and libration amplitude ϕ_0 for the specified r_{ICB} and χ_{Si} values.

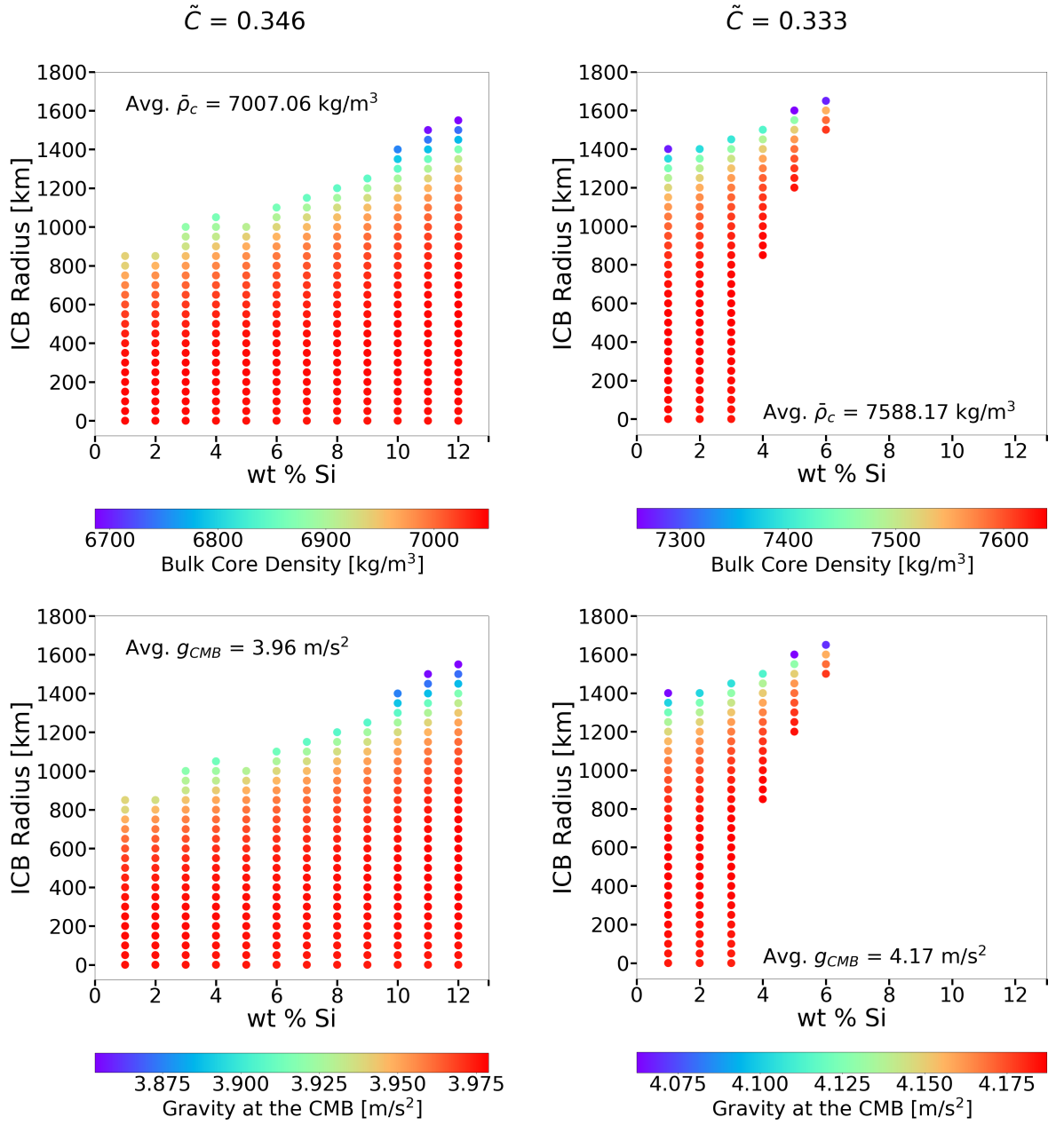


Figure S2. Bulk core density (top) and gravity at the CMB (bottom) for the mean high (left) and low (right) MoI constraints. Absence of a symbol indicates that it is not possible to match the combination of $\tilde{C}$, mass M , and libration amplitude ϕ_0 for the specified r_{ICB} and χ_{Si} values.

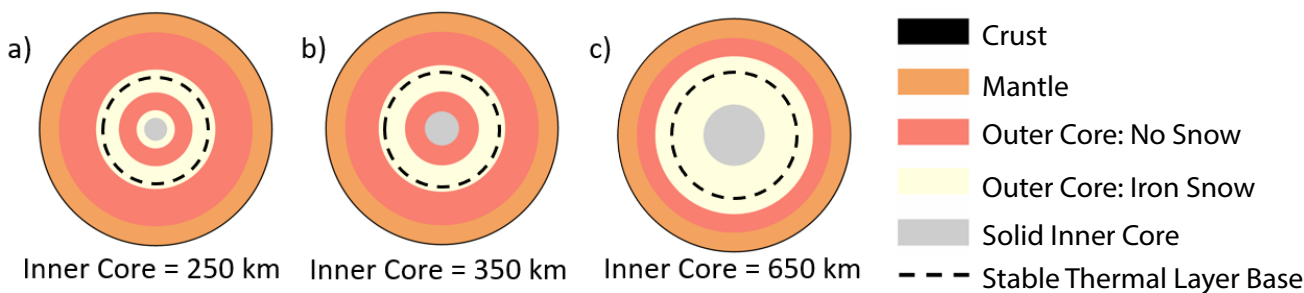


Figure S3. Examples of the different snow zone regimes for interior models with 1 wt% Si and different inner core sizes that match the high MoI constraint. From left to right, the regimes are (a) “deep snow + layers”, (b) “layers”, and (c) “deep snow”. Internal layers are labeled in the legend, and the black dashed line shows the boundary (halfway through the liquid outer core) for the base of the thermally stratified region. Dynamo action driven by iron snow is possible in the first two snow regimes.

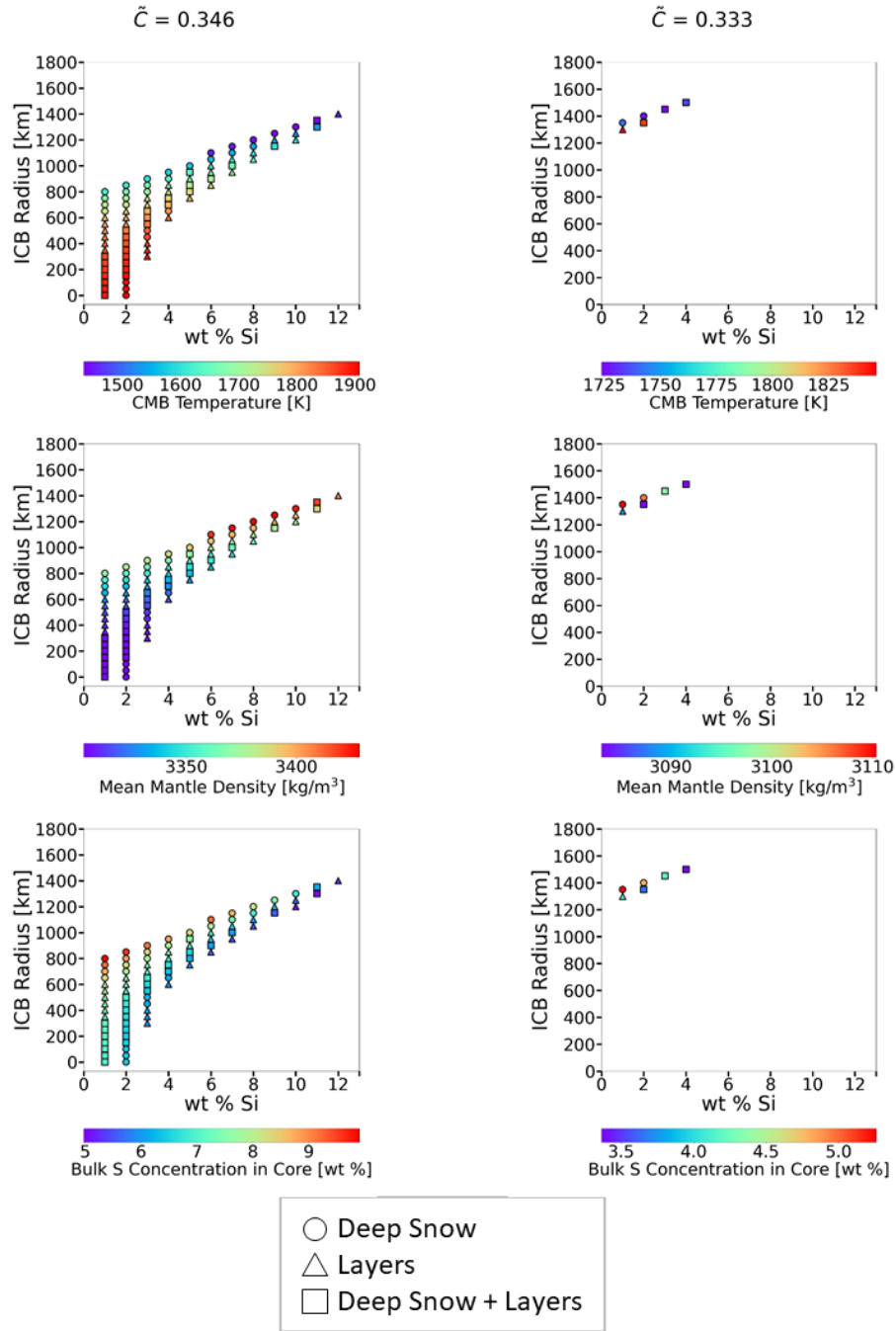


Figure S4. Categorization of iron snow regimes as a function of (top) CMB temperature, (middle) mean mantle density, and (bottom) bulk sulfur concentration for interior models with r_{ICB} and χ_{Si} values that satisfy the high (left) and low (right) MoI constraints. Symbols (indicated in the legend) identify the iron snow regime within each model.

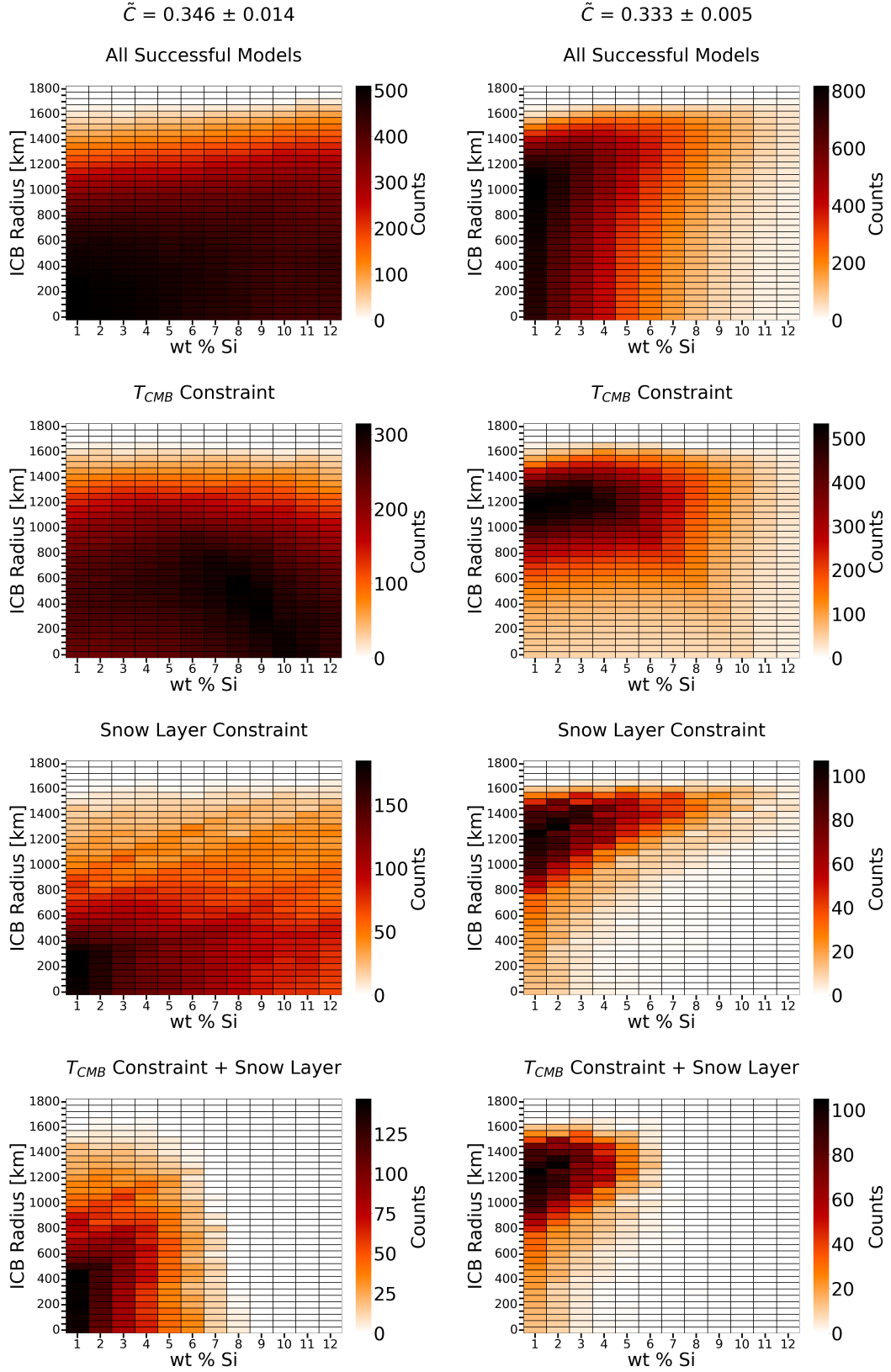


Figure S5. Probability distributions of r_{ICB} and χ_{Si} from interior models sampled from the high (left) and low (right) MoI constraints.

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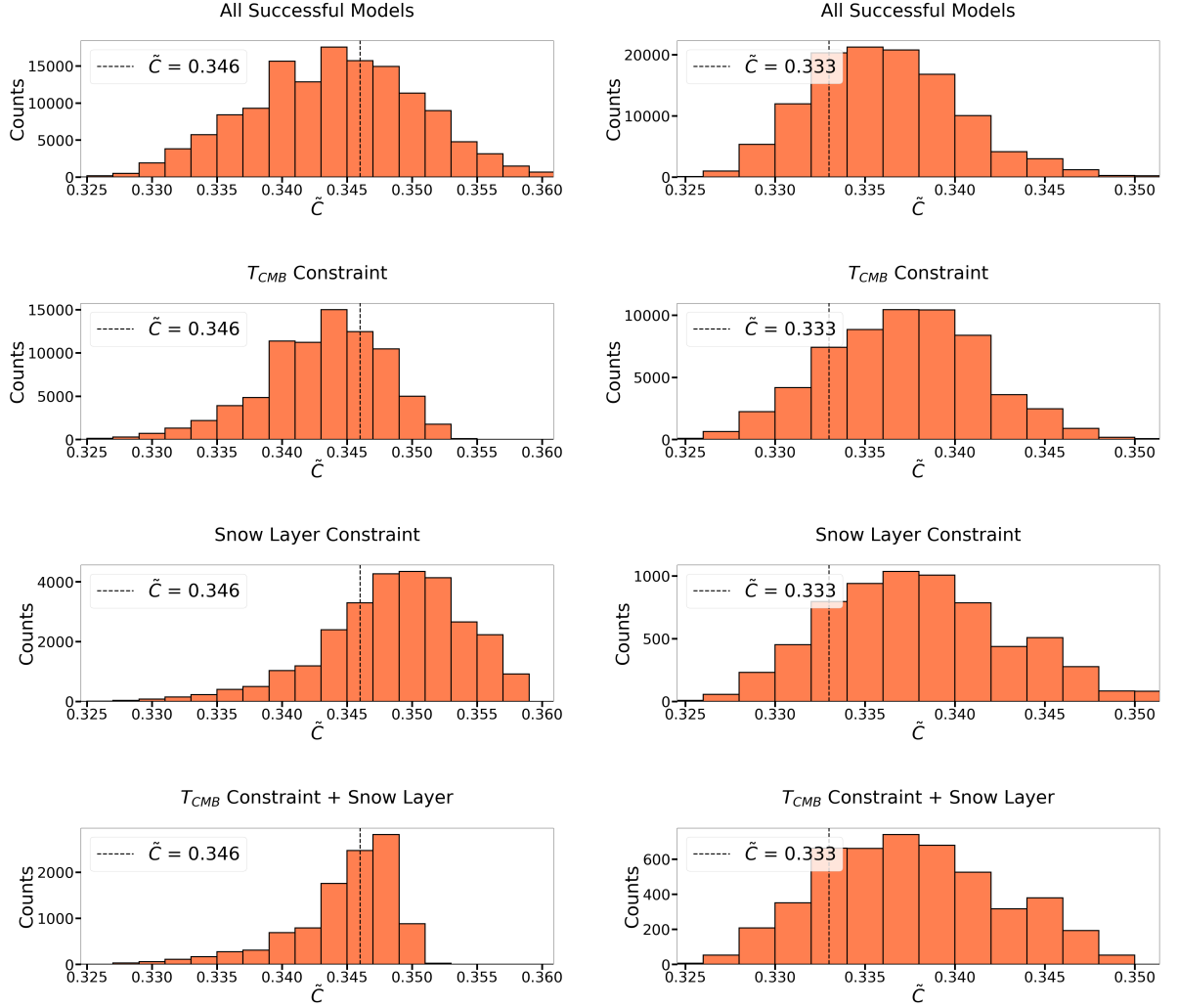
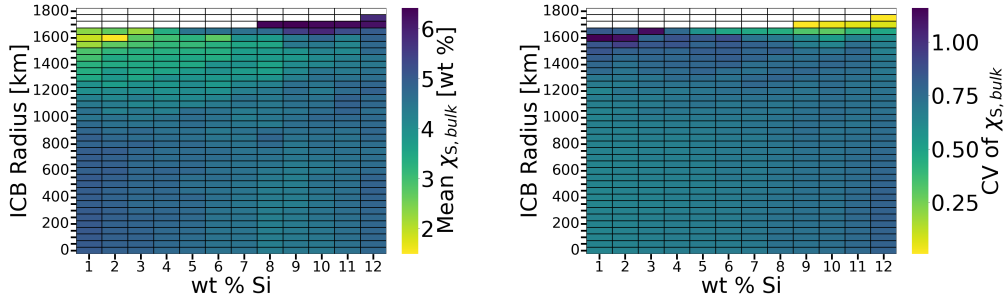


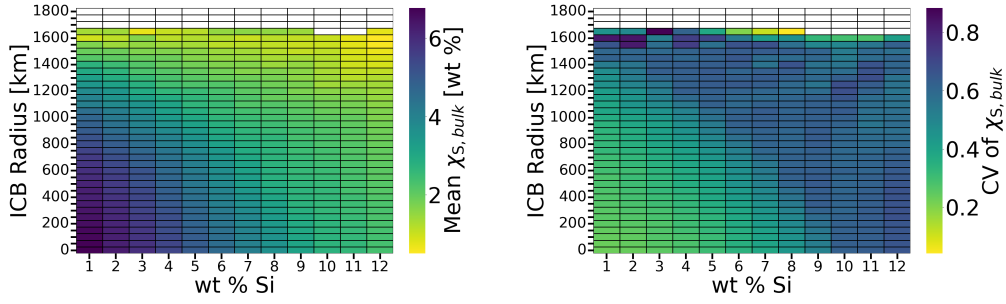
Figure S6. Probability distributions of $\tilde{C}$ for the models shown in Figure S5 selected from the high (left) and low (right) MoI constraints. The bin size of the histograms is 0.002.

$$\tilde{C} = 0.346 \pm 0.014$$

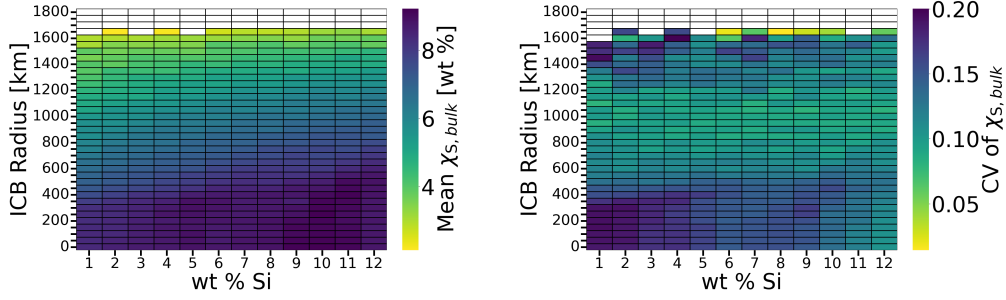
All Successful Models



T_{CMB} Constraint



Snow Layer Constraint



T_{CMB} Constraint + Snow Layer

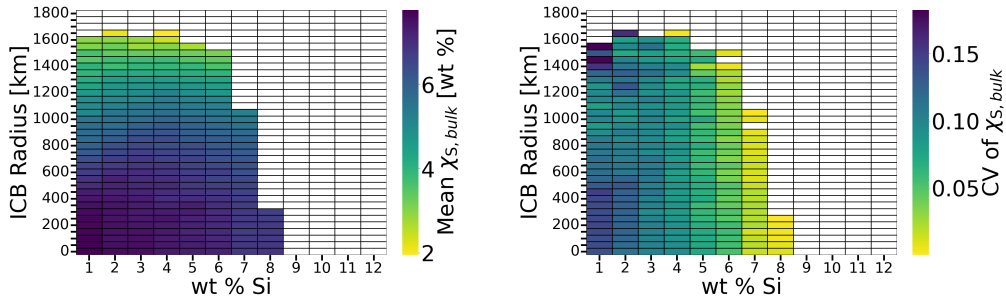
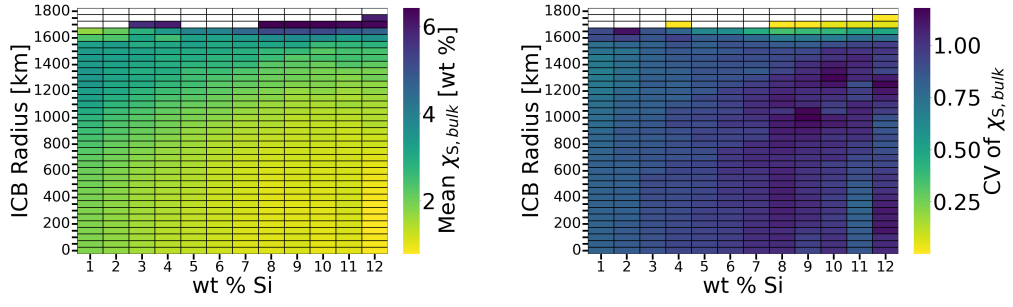
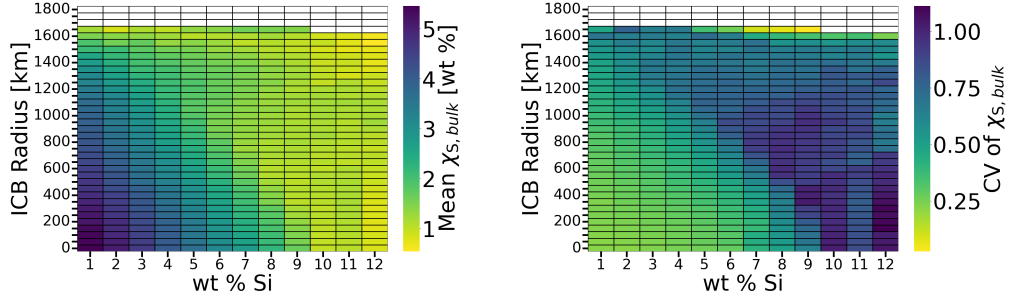


Figure S7. The mean values (left) and coefficients of variation (CV, right) of the bulk weight fraction of S in the core from models selected from the high MoI constraint. Cases where a mean $\chi_{S,bulk}$ does not have a corresponding CV value indicate a sample size of 1.

$$\tilde{C} = 0.333 \pm 0.005$$

All Successful Models

 T_{CMB} Constraint

Snow Layer Constraint

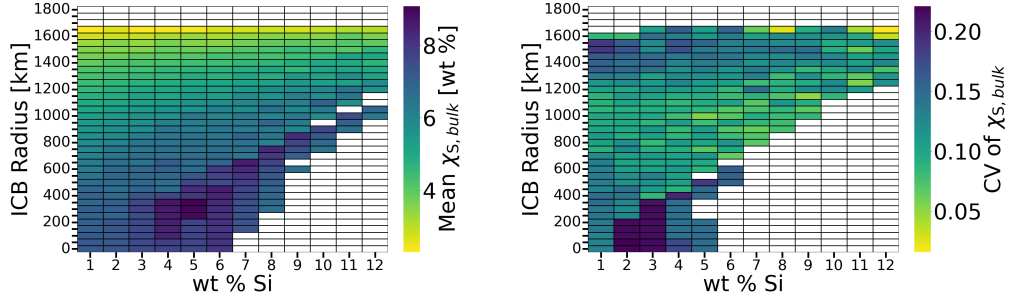
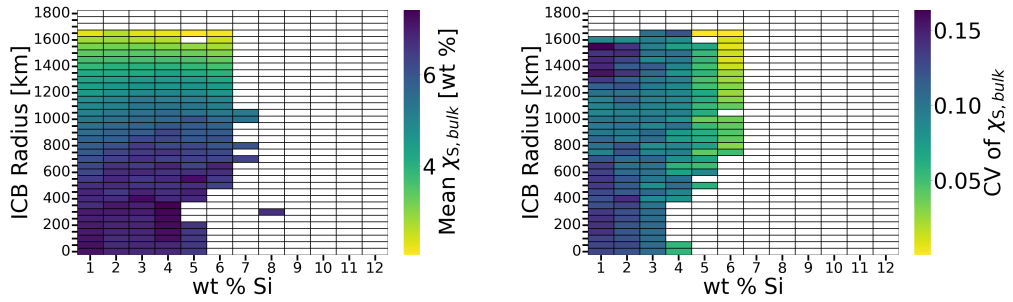
 T_{CMB} Constraint + Snow Layer

Figure S8. The mean values (left) and coefficients of variation (CV, right) of the bulk weight fraction of S in the core from models selected from the low MoI constraint. Cases where a mean $\chi_{S,bulk}$ does not have a corresponding CV value indicate a sample size of 1.

$$\tilde{C} = 0.346 \pm 0.014$$

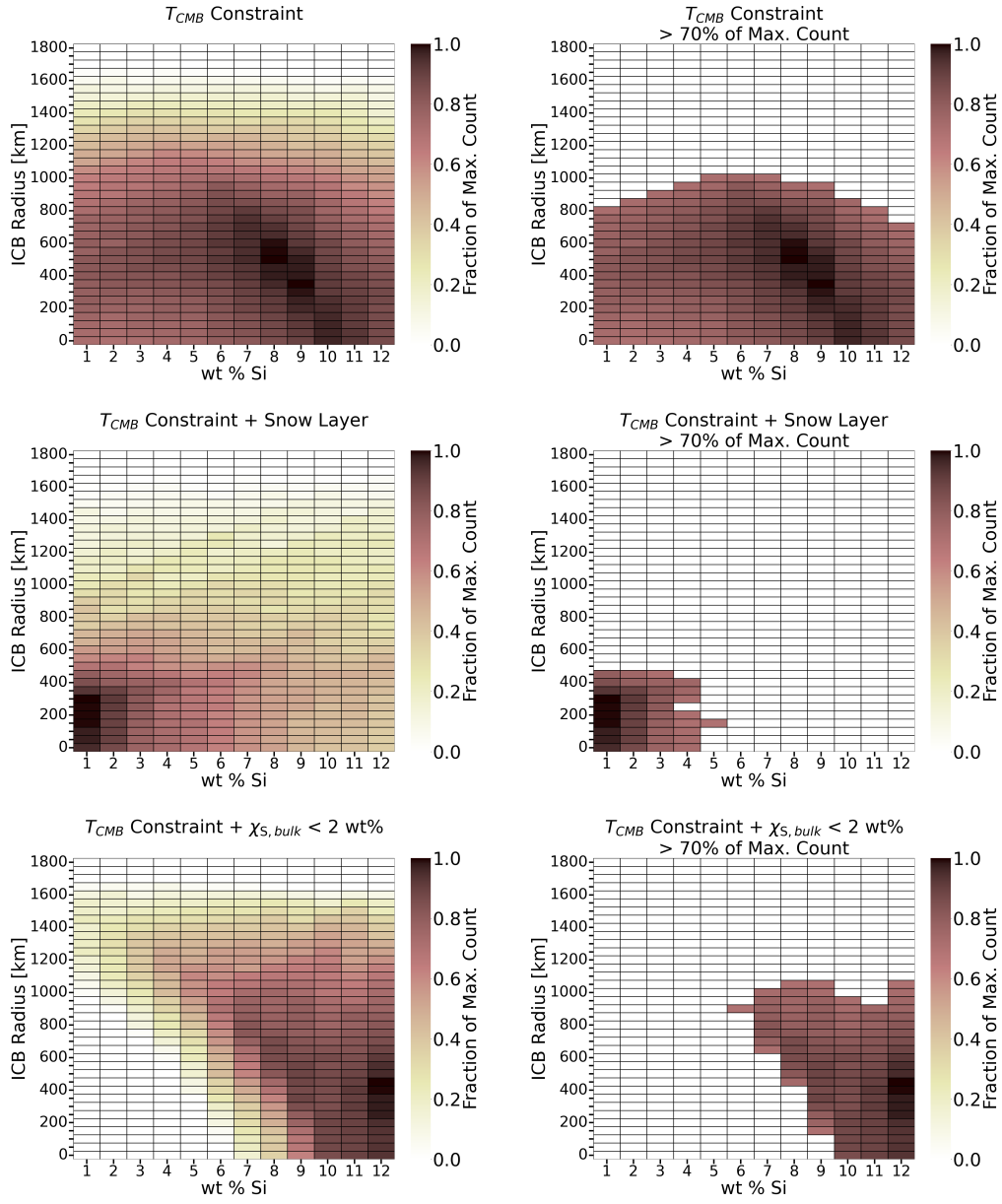


Figure S9. Probability distributions of r_{ICB} and χ_{Si} for the high MoI constraint, represented as fractions of the maximum counts. The left panels show all fraction values, while the right panels show only the fractions that are equal to or exceed 0.7. Samples correspond to the left columns of Figures 1, 2, and 4 of the main text.

$$\tilde{C} = 0.333 \pm 0.005$$

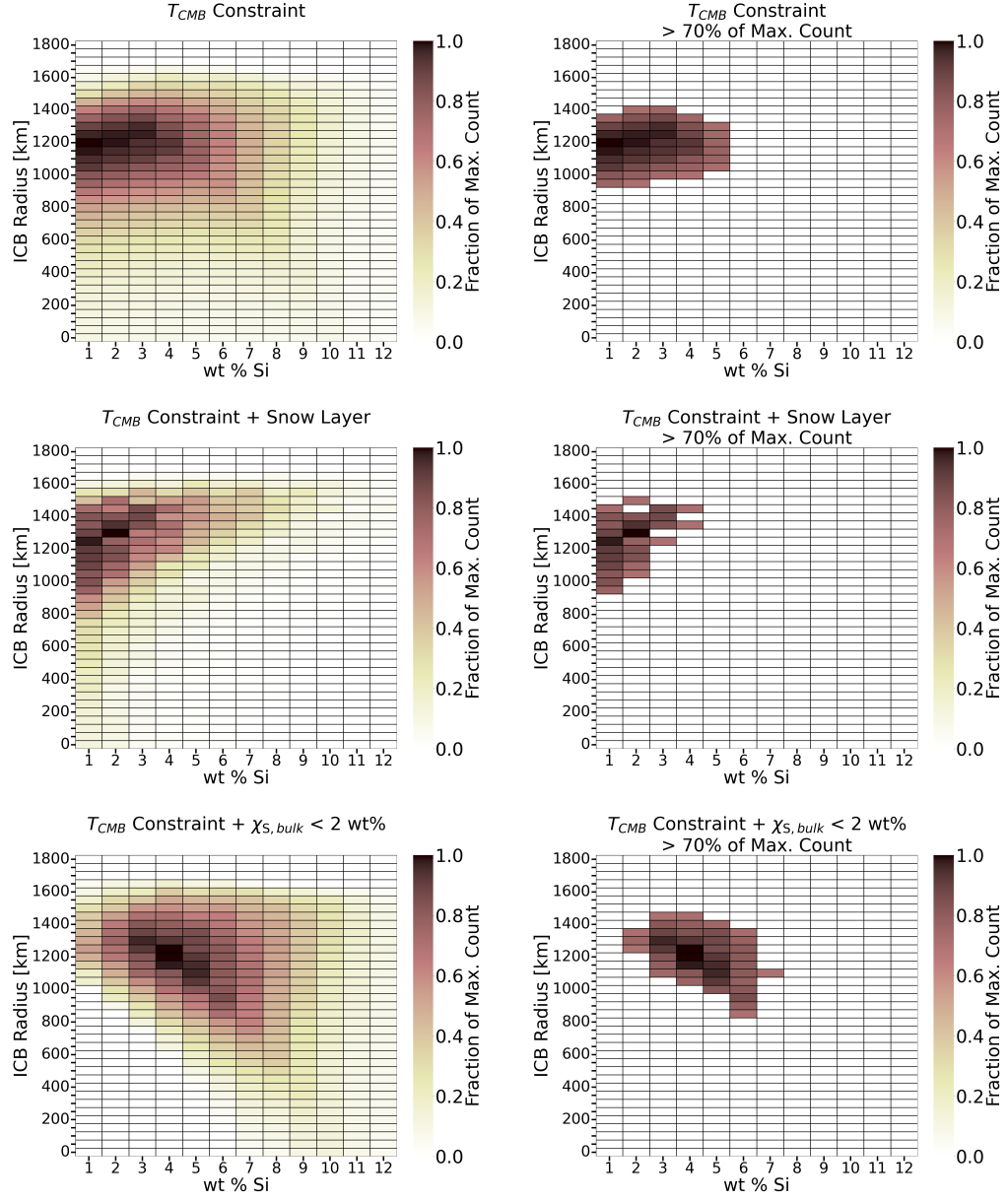


Figure S10. Probability distributions of r_{ICB} and χ_{Si} for the low MoI constraint, represented as fractions of the maximum counts. The left panels show all fraction values, while the right panels show only the fractions that are equal to or exceed 0.7. Samples correspond to the right columns of Figures 1, 2, and 4 of the main text.