

RC2

We would like to thank the reviewer for their constructive suggestions. The typographical errors will all be corrected, and we plan to make the following changes to the manuscript based on the feedback:

[reviewer comments in blue font, replies in black font]

1. I found the role of the thermodynamic (K_{D^O}) model of Frost et al. (2010) in the PlanetBuilder solver somewhat difficult to understand.

As I understand the procedure, PlanetBuilder first calculates a hypothetical equilibrated composition from the mass-balance and metal–silicate partitioning equations. The resulting (K_{D^O}) is then compared with the thermodynamically calculated (K_{D^O}) from Frost et al. (2010), and the FeO abundance is adjusted until the two values agree.

Could the authors explain more explicitly why this two-step approach is used? In particular, what is the conceptual or computational advantage of deriving (K_{D^O}) from the PlanetBuilder composition and then using the Frost et al. (2010) thermodynamic calculation as an independent equilibrium constraint, rather than formulating the thermodynamic equilibrium condition directly together with the mass-balance and partitioning equations? I do not necessarily suggest that the present approach is incorrect. Rather, I think the rationale for this architecture should be made clearer, particularly because the Frost et al. (2010) model appears to provide the thermodynamic equilibrium condition for oxygen partitioning.

The two-step approach was initially introduced in Rubie et al. (2011). We implemented it to have an independent verification of the oxygen partitioning that is thermodynamically correct. Major elements such as Ni and Si have experimentally tested KD parametrisations based on PT conditions that can be used to determine partitioning behaviour prior to equilibration. Oxygen does not have such a parameterisation or constraint. Instead, the oxygen concentrations and partitioning behaviour must be derived during the equilibration, unconstrained by pressure and temperature, using only the composition (see Eq. 16 and 44). The model from Frost et al. (2010) provides an independent thermodynamic constraint for the oxygen concentrations to ensure the K_{D^O} and concentration of oxygen are realistic for the specific composition and conditions.

We chose to keep the two methods of deriving K_{D^O} separate for computational reasons:

1) We use the limited, and free version of MIDACO. This version can have up to seven simultaneous constraints for a solver, and the calculations for the PlanetBuilder composition already uses all seven. This complicates merging the two methods. 2) The K_{D^O} of Frost et al. (2010) is used inside the larger solver for the PlanetBuilder composition. This means that the entire MIDACO solver for Frost et al. (2010) is completed within one iteration of the MIDACO solver for the planetary composition and repeated in the next iteration. Merging the two methods would likely slow the program down without additional investment into optimisation.

We will adjust the main text to clarify the role of the thermodynamic Frost model.

2. There appears to be a possible inconsistency between the description of the solver and Fig. 2B–G.

The manuscript states that the seven unknown variables are “solved simultaneously”.

However, the subsequent description states that the solver first selects a value for the FeO abundance in the planetary mantle, which is then used to derive the other abundances from the mass-balance and metal–silicate partitioning equations. This latter description, together with Fig. 2B–G, appears to suggest that the abundances are derived sequentially.

Could the authors clarify whether all seven variables are actually independent variables optimized simultaneously by MIDACO, or whether FeO is the only variable directly varied by the solver and the other abundances are subsequently derived from it?

If the latter is the case, I suggest revising the wording in Sect. 2.3. The seven quantities may constitute the unknown abundances of the final equilibrium state, but they would not necessarily be seven independent optimization variables.

Clarifying this point would also make Fig. 2B–G considerably easier to understand.

We acknowledge that the wording was poorly chosen, and will take steps to improve it in the Sect. 2.3. It is correct that the FeO is the only variable that is directly adjusted during every iteration, and the other variables are derived from the FeO value. However, all seven variables have to be within the constraint limits for the composition to be accepted.

3. The use of a single effective pressure and temperature for each accretion step is a reasonable modelling simplification, but it is potentially important because the partition coefficients are strongly dependent on pressure and temperature.

Could the authors discuss more explicitly how the choice of effective P–T conditions affects the model results? If possible, a sensitivity test using plausible variations around the adopted effective P–T conditions, or a P–T contour plot showing the resulting partition coefficients, would help quantify the importance of this approximation relative to the effects of the partitioning parameters and metal activity corrections.

For this manuscript, we used the effective P–T conditions from Rubie et al. (2011). While investigating the effect of changes in the P–T conditions is important, that is outside of the scope of this manuscript. We will specifically discuss the effect of pressure and temperature in a follow-up paper that is being prepared for publication.

4. The claim of “excellent agreement” with Rubie et al. (2011) (Sect. 3, l. 432–433) may be somewhat overstated. As shown in Supplementary Material S2, there are noticeable discrepancies between the PlanetBuilder results and those of Rubie et al. (2011), particularly for core O and, to a lesser extent, core Fe. The discrepancy in core O reaches approximately 30% relative to the Rubie et al. (2011) result.

I recognize that the authors discuss possible sources of these differences in the Supplementary Material, however, given their magnitude, I think they should be quantified and acknowledged more explicitly in the main text. Could the authors clarify whether they consider these differences sufficiently small to justify the description of “excellent agreement”?

Our claim for the excellent agreement comes from PlanetBuilders ability to replicate the Rubie et al. (2011) data when using the exact same equations as used by Rubie et al. (2011).

We validated our code directly with the code from Rubie et al. (2011). However, Rubie et al. (2011) used an adjusted version of the Frost et al. (2010) equations (Eq. S.2) to calculate the thermodynamic K^D_O (step J in Figure 2). These adjustments simplified the thermodynamic expression and enabled Rubie et al. (2011) to approximate the K^D_O with an incremental approach with step-halving to enforce positive values. PlanetBuilder uses the equations as presented in Frost et al. (2011) without this simplification step, combined with a second MIDACO solver to acquire more precise K^D_O values. As the thermodynamic K^D_O calculations are directly used to verify the K^D_O from the composition (Fig 2.K), this directly affects the resulting concentration of O in the core, and to a lesser extent the Fe in the core. Other elements are affected as well, but only indirectly. We agree with the suggestion that an approved explanation in the main text is required and will adjust it in Sect. 3.