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Interactive comment on "Timescales of chemical equilibrium between the convecting solid mantle and over-/underlying magma oceans" *by* Daniela Paz Bolrão et al.

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Response to the Reviewers and Editor

We would like to thank the Editor for handling our paper and the Reviewers for taking the time to review our manuscript so thoughtfully. We took the useful comments and pertinent questions into consideration, which have substantially improved our paper. Both reviewers address an important point regarding the value of the Buoyancy number, B. We agree that the value used in our simulations (1.0) is lower than a realistic value (3.0 or more), and we decided to show results for a more reasonable value of B. Therefore, at the moment we are trying to run new simulations with a proper value for B. Unfortunately, we don't have the new results yet since our clusters are still facing problems from a cyber attack that occurred late-May. We plan to have the results in the next couple of months.

Therefore, we would like to ask if it possible to have an extension of two months, to address the B problem properly. The rest of our responses are reported below.

Response to Reviewer Number 1

General comments

Reviewer: My main concern is about the treatment of chemical buoyancy. While the results on chemical equilibration are relevant for all sorts of species affected by fractionation (volatiles, heat-producing elements, trace elements etc.), the framework of this work is that of Fe fractionation, which has an impact on the dynamics of the system by inducing density anomalies. This is accounted for in the model. However, the effects of compositional buoyancy on the flow are not discussed. Furthermore, the density difference between the two compositional end-members considered being probably uncertain (the two-component model itself being a simplification), I would have expected this density difference (i.e. the buoyancy number) to be one of the parameters of the study. Yet only one value is considered, and is not even motivated. Actually, doing a quick calculation with $\alpha = 2 \times 10^{-5}$ K^{-1}, $\Delta T = 2000$ K (typical value for the geometry used here with the melting curves from Fiquet et al., 2010 for the initial temperature profile), $\rho_{mantle} = 4000$ kg/m^3 (as in Ballmer et al., 2017) and B=1 (the value used in the present work), I found: $\Delta\rho = \alpha \Delta T B \rho_{mantle} = 160$ kg/m^3, which is about one order of magnitude lower than what you would expect for pure FeO and pure MgO end-members (e.g. Boukaré et al., 2015). Therefore I think the authors should either more strongly motivate their choice of B=1, or consider testing several values for it. For instance, using B=0, they could extend their discussion to strictly passively advected material, like trace elements.

→ **Authors:** Indeed the value of B is lower than expected for Earth. We did not vary the value of B because our parameter space was already too vast. We decided to keep B = 1.0 because our preliminary results showed that B does not have a huge impact on the dynamics of the solid mantle. However, we agree that in order to avoid confusion is probably better to show results for a more reasonable value of B. Therefore, at the moment we are trying to run new simulations with B = 3.0 (this value comes from $B = \frac{\Delta\rho_{ch}}{\alpha \Delta T \rho_0} = \frac{670}{0.00002 \times 3000 \times 4000} = 2.8$). Unfortunately, we don't have the new results yet. Our clusters are still facing problems from a cyber attack that occurred late-May. We plan to have the results in the next couple of months.

Specific comments

Reviewer: Lines 37 and 46: I am a bit confused here: the opening and concluding sentences "the solidus is steeper than the isentrope" and "the adiabat is steeper than the melting curve" seem contradictory. If you do mean the that the adiabat is steeper than the melting curve (which you need for re-melting of sinking, Fe-rich cumulates), it seems to me that you are already in the middle-out crystallization case. Or do you expect the adiabat to be steeper than the melting curves only in the solid mantle?

→ **Authors:** We decided to change the sentence in the text.

Reviewer: Figure 1: Although it is made clear that the curvature of the liquidus curve in panel b is exagerated, I am a bit puzzled by the fact that the temperature decreases in the bottom of the mantle, rather than only increasing at a lower rate than the adiabats. I don't think anyone predicts that the temperature of the melting curves actually decrease with depth (it just increases at a lower rate than the adiabat).

→ **Authors:** We agree it is not the best representation. It seemed to us that in order to draw a basal magma ocean, we would have to exaggerate the curvature of the liquidus. We put more thought into this figure and we changed it in a way that the temperature of the liquidus increases at a lower rate than the adiabats. The new figure is now included in the paper.

Reviewer: I do not understand if the computing mesh changes with the geometry of the case: although it is suggested in Figure 2 (with varying R+ and R-), I don't really see it in Figure 5 (but maybe the outer-to-inner radius differences between those cases are too small, in which case that might be notified in the caption).

→ **Authors:** Meshes are indeed different, however, differences between the aspect ratio of case are too small to be noticed (differences are only obvious if one makes use of a ruler). We agree that this is a point that should be addressed to avoid confusion. We modified the caption of figure 5 and added this note.

Reviewer: Please, include a table with the values of the different parameters and quantities used: hTMO, hS, hBMO (and related R+/R- if relevant), Ra (and/or SC and Rac), B, $\Phi^{\pm}$, K, X_{bulk}^{Fe}.

→ **Authors:** Included.

Reviewer: Line 86-87: "We ensure mechanical stability between the solid mantle and magma oceans, i.e., $\rho_{TMO} < \rho_S < \rho_{BMO}$". How do you do that? As far as I understand, density is only parametrized by XFe, and when you reach equilibrium, both TMO and BMO have the same XFe which should imply: $\rho_{TMO} = \rho_{BMO}$. But anyway the density of the magma oceans is not considered in this study (there is no other reference to ρ_{MO} in the text except in Fig. 2), so this sentence might be superfluous.

→ **Authors:** It is a good point. This is just a misuse of the word "ensure" from our part. We assume this mechanical stability condition holds true (and physically, it is necessary for Φ to be positive). We changed the word "ensure" to "assume" for clarity.

Reviewer: Lines 143-146: This fact is important and would deserve attention (in future studies). The melt/freeze boundary conditions have been developed to study the inner core boundary where a unique melting temperature can be defined. For mantle rock, as pointed out in the text, the temperature span between solidus and liquidus probably induces different behavior, which is hard to tell a priori.

→ **Authors:** It's a good point and indeed this should be taken into account in future projects!

Reviewer: You assume that at equilibrium, XFe in the solid is homogeneous, but I can imagine that overturn of heavy cumulates could result in a layered configuration and an associated layered convection pattern where FeO would be sequestered at the bottom, resulting in a Fe-rich BMO, a Fe-poor TMO, and heterogeneous (layered) mantle.

→ **Authors:** We do not assume that XFe in the solid is homogeneous. We show that although average composition of the solid mantle tend to mutual chemical equilibrium, chemical homogeneity across the solid mantle is not necessarily reached (figure 4). As the reviewer points out, the solid mantle ends up strongly heterogeneous (albeit without layering), and the implications are discussed in the paper. Instead, the timescale of "half-equilibration" provides a measure of significant chemical changes in the magma ocean relative to the *average* mantle. We now explain this more clearly in the text. The thermo-chemical evolution anticipated by the reviewer (in terms of layering) is not predicted by any of our models (and again nothing is imposed that would prevent such an evolution). In a current study (in prep.), we explore the effects of initial mantle stratification in the

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solid (while the TMO/BMO are still present), but the related consequences go beyond the scope of this paper.

Reviewer: A few more words about how particles are handled would be welcome. For generalities (e.g. advection algorithm), references to previous work would be sufficient, but I guess new techniques were introduced for this study, whose description could benefit to the community. In particular, how do you ensure the mass conservation with permeable boundaries: do you balance the number of particles going out at the “melting” interface with that coming in at the “freezing” one? And how do you distribute the incoming particles?

→ **Authors:** This deserves attention indeed. We changed the explanation in "2.3 Compositional treatment" to address this point. We simulate melting of solid material when dynamic topography develops outside the solid domain, i.e., when there is an outflux of material of the solid domain. Melting is simulated assuming that no fractionation operates when the solid melts, i.e., all (Fe,Mg)O present in this topography goes into the magma ocean. Therefore, tracers that leave the domain pass their information (about mass and composition) to the magma ocean, and are deleted. We simulate crystallisation of the magma ocean when negative dynamic topography develops in the solid domain. When this happens, cells near the boundary are left with no tracers, so new tracers have to be introduced in those cells. These new tracers simulate solid being created. We calculate the influx of mass corresponding to this dynamic topography, and distribute this mass to the new tracers. The composition of the solid created is related to that of the liquid by fractional crystallisation. Therefore, only a fraction of FeO goes into the solid, and this fraction is given by the partition coefficient, K.

Reviewer: Figure 4: Decimals in non-dimensional time are superfluous. Moreover, since the convection is mainly thermal, having snapshots of the temperature could help, especially for the case with a low value of Φ, since it is an unusual convection pattern. If you do, you might consider discarding some timesteps which are not so important to understand the evolution, in order save space on the figure.

→ **Authors:** Regarding "Decimals in non-dimensional time are superfluous", we agree and modified the figure to reduce the number of decimals. Regarding the temperature snapshots: we will add them once we have new results.

Reviewer: The half-equilibrium time is parameterized using the parameters of the study: Ra, Φ and VS/VM. It would be interesting to discuss what might be the influence of other parameters that where not varied in this study (e.g. the buoyancy number, the partition coefficient or the bulk XFe).

→ **Authors:** As mentioned previously in this document, simulations at $B = 3$ are ongoing. The partition coefficient is not expected to affect results tremendously when varying in its fairly narrow range of realistic values. It is harder to predict the effect of the bulk XFe, and in particular how it is distributed between the solid and the ocean(s) in the initial condition. We chose here to focus on the consequences of the phase change boundary condition to show it is an important ingredient when considering the chemical evolution of our system. We do agree that it would be important to study the effect of the initial condition, but we think it is out of scope of this paper, and better suited in more realistic studies about the long term evolution of the solid/magma ocean(s) system.

Reviewer: Figure 7 is hard to read, and largely redundant with Figure 6. One important new information is that increasing Φ increases the influence of the volume of the solid mantle, but it is already mentioned in the text. If the point is to represent the good agreement of the scaling law with the predictions, I think Figure A1 is sufficient.

→ **Authors:** We agree that figure 7 may be too complicated due to the amount of information. We remove figure 7 from this manuscript, since the main information is written in the text, and the good agreement of the scaling law with the predictions is made in figure A1.

Reviewer: Several more recent studies on the timescale for crystallization of a terrestrial magma ocean have been published since Lebrun et al. 2013: – Salvador et al., The relative influence of H2O and CO2 on the primitive surface conditions and evolution of rocky planets, JGR: Planets 122, 2017. – Nikolaou et al., What factors affect the duration and outgassing of the terrestrial magma ocean? ApJ 875, 2019.

→ **Authors:** Unfortunately these citations were missing in the first version of this manuscript. We acknowledge the work made by Salvador et al. and Nikolaou et al. and correct the mistake in this new version of the paper.

Reviewer: In the discussion you suggest that Φ is low when the crystallization starts (line 309), and that $\Phi \sim 100$ is a “realistic value” (line 382), but there is no discussion on the expected evolution of Φ, so you should at least cite some previous studies where it is explained.

→ **Authors:** We make a note in the methodology section that Morison et al. (2019) and Morison (2019) estimated $\Phi^+ \sim 10^{-5}$ and $\Phi^- \sim 10^{-3}$, for a purely thermal case. So small values of Φ are expected for the Earth. However, our paper includes a compositional treatment, and given that $\Phi^\pm$ is difficult to constrain, we vary this value between 10^{-1} and 10^5 (we use $\Phi^\pm = 10^{-1}$ as the lowest value possible for $\Phi^\pm$ because the resolution of the thermal boundary layer is computationally demanding once $\Phi^{\pm}$ decreases below 10^{-1}). Later in the conclusion we mention $\Phi \sim 100$ is a “realistic value” and this may be confusing indeed. What we meant is that low values of Φ are expected (Morison et al. (2019) and Morison (2019)), and we show that at any value below $\Phi^{\pm} \sim 100$, the system reaches chemical (half-)equilibration before magma ocean crystallisation (previous figure 8, now figure 7). We changed this sentence to "Moreover, this efficient transfer of FeO renders the timescales of chemical (half-)equilibration between the solid mantle and magma ocean(s) shorter than (or on the order of) 1 Myr."

Reviewer: I don’t really understand the fitting algorithm: Do you scan all parameters at once, or do you fit them one after the other? Do you choose which branch of the scaling law (i.e. which set of parameters) is fitted depending on the location in the parameter space (i.e. implying the regime boundary)? Since it is an appendix, I think you might develop this (very succinct) description, or even write the algorithm as pseudo-code if it is not too long. It would be also a good place to define what you call “error” in Table 1.

→ **Authors:** This is a good point and we explain it better in the appendix now. All parameters are scanned at the same time until one solution is found. Once the solution is found the window search of each parameter is redefined to values closer to the value found. This process is done multiple times, to refine the solution.

Technical corrections

Reviewer: âĂć Line 26: “crystals start to appear and consolidate...” âĂć Line 42: “.. become denser with time.” You could refer to Figure 1a where this process is represented. âĂć Line 58: As for Line 42, I would also refer to Figure 1b. âĂć Line 118: “is noted τ_η” rather than “is given by τ_η”. âĂć Line 160-161: Depending on what you mean, I would rather write that “FeO and MgO are thought to be the Fe-rich and Mg-rich end-members of mantle silicates” or that “FeO and MgO represent the Fe-rich and Mg-rich end-members of mantle silicates”. âĂć Line 172: “(similar to a half-life)” I would introduce the notion of half-equilibrium after calculating the equilibrium. âĂć Line 194: I think the correct word here is “bounded” (as you use it further). âĂć Line 208: “. . . in dimensionless time units...” âĂć Line 210: “. . . thereby bringing the solid mantle and the TMO close to chemical equilibrium” âĂć Line 213: since you’re giving the half-equilibrium times in non-dimensional units, which are not very insightful, it might be better to compare these times between each other (e.g. saying that half equilibrium is reached for $\Phi = 10^{-1} \sim 10$ times faster than for $\Phi = 10^2$, and ~ 200 faster than for $\Phi = 10^3$). âĂć Line 214: “... for these three cases.” or “... for these three values of Φ^- âĂć Figures 4 and 5: What sets the streamlines’ color-code? Maybe having them just white would avoid confusing with FeO content in the cases where mixing induces small-scale heterogeneites. âĂć Line 249: Shouldn’t it be a minimum rather than a maximum? âĂć Caption Figure 6: “white circles” instead of “white colours”. âĂć Table 1: It is not clear to me what the “error” is in this context. âĂć Line 257: “Our models predict that in the regime of efficient material transfer (i.e., for low values of Φ), timescales to reach chemical half-equilibrium are virtually unaffected by the volume of the solid mantle” I would then expect a3 to be close to 0, why is it not the case? âĂć Line 270: “Agrusta et al., 2019 showed” âĂć Line 303: Whether or not chemical equilibration occurs between the solid mantle and magma ocean(s) is highly influential on the extent of this initial chemical stratification.” C7 âĂć Line 328-329: “Note that the thermal inertia of the core is similar to ...”

→ **Authors:** All these comments are very useful and we tried to address them all in the text.

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Response to Reviewer Number 2

Specific comments

Reviewer Point 1: Thermo-chemical convection: The number of buoyancy is set to 1 without further explanation. Why was this value taken and how does the choice of B influence the results? With the present values it seems that the chemical density variation has no significant influence.

→ **Authors:** Indeed the value of B we use is lower than what is expected for Earth. We did not vary the value of B because our parameter space was already too vast. However, we agree that it is probably better to show results for a more reasonable value of B. Therefore, at the moment we are trying to run new simulations with B = 3.0 (this value comes from $B = \frac{\Delta\rho_{ch}}{\alpha\Delta T\rho_0} = \frac{670}{0.00002\times3000\times4000} = 2.8$). Unfortunately, we don't have the new results yet. Our clusters are still facing problems from a cyber attack that occurred late-May. We plan to have the results in the next couple of months.

Reviewer Point 2: In the initial setup a homogeneous FeO content of solid mantle and magma ocean is assumed. As the authors themselves write, this is not a realistic initial state but it also not clear how sensible are the obtained time scales depending on initial conditions? In the current setup, the material that forms in the topography depression is depleted in FeO, this would not be the case for a more realistic start condition. An initial unstable gradient in the solid mantle can trigger convection but may also result is a stable configuration after overturn, depending on B (see above). This can be important for the time scale of chemical equilibrium - if in this case a chemical equilibrium can be established.

→ **Authors:** This is a good point. In the new simulations that are currently

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running with $B = 3$, we also use a more realistic initial condition which leads to material enriched in FeO in newly formed solid. Overall, it is difficult to fully assess how the initial condition would affect results, especially as this makes the parameter space much larger. We chose here to focus on the consequences of the phase change boundary condition to show it is an important ingredient when considering the chemical evolution of our system. We do agree that it would be important to study the effect of the initial condition, but we think it is out of scope of this paper, and better suited in more realistic studies about the long term evolution of the solid/magma ocean(s) system.

Reviewer Point 3: Two effects have been neglected, but they can also result in chemical equilibration and compositional mixing before final magma ocean crystallization: 1) When the solid mantle grows and has no fixed boundaries, as is assumed here, convection causes the new top crystallized layer, which should have a different FeO content, to sink and mix continuously with the solid mantle. 2) If convection in the solid mantle starts before the solidification of MO, partial melting of the cumulates and 'feeding' of the MO with this melt is very likely. Both effects change the chemical equilibrium considerably and do not necessarily require the material to be able to flow through by phase change. However, the latter may further reduce the time scale of chemical equilibrium.

→ **Authors:** These are two important points and we modified the manuscript to address them. Regarding the first one: in this paper we assume fixed boundaries and test different thicknesses of the solid mantle (or magma oceans). Indeed a moving boundary would create a new top crystallised layer, which should have a different FeO content, and sink and mix continuously with the solid mantle. This effect could result in chemical equilibration and compositional mixing before final magma ocean crystallisation. However, we show here that with the phase change boundary condition, chemical equilibration can occur on a timescale that is much smaller than that of crystallization. Integrating the effect of the moving boundary is much more demanding computationally (an evolution model for magma oceans is necessary, as well as some way to deal with moving boundaries). This will be the subject of more complete studies in the future. Note also that in this study we take Φ as being constant through time, but because this number depends on the dynamics and thicknesses of the magma oceans, Φ may change continuously in a more realistic model with moving boundaries. Variations of Φ and a moving-boundary scheme should definitely be considered in further studies to study the long-term evolution of the solid/magma ocean(s) system.

Regarding point 2: in this study we focus our attention to a phase change boundary condition, that allows material to flow through the boundary and continuously change the composition of solid and liquid reservoirs. Partial melting of solid cumulates can indeed still change the composition of the magma ocean, without the use of this boundary condition. However, we show that with this boundary condition a larger volume of material can (re-)melt and crystallise efficiently at either or both solid-liquid phase boundaries.

Reviewer Point 4: Steady-state simulations, i.e. delta T is constant, but also no internal heat sources and a constant viscosity are used – all these effects can influence the strength of convection (and chemical equilibration) and possibly the convection pattern. In particular the influence of internal heat and a temperature dependent viscosity could be tested fast.

→ **Authors:** Indeed these effects can influence the results. But testing the effect of internal heat sources, as well as temperature dependent viscosity, goes beyond the scope of the current paper. These should be definitely taken into account in future projects.

Reviewer Point 5: A new phase change boundary condition for convection has been investigated, are there benchmark studies also for sufficient resolution or how do the authors ensure that the calculations are correct?

→ **Authors:** The phase change boundary condition implementation was tested against linear stability analysis (Agrusta et al., 2019 for cartesian geometry; Morison, 2019 spherical geometry). In this study we also check energy conservation over the solid mantle, and iron mass conservation over the whole mantle (solid mantle and magma oceans).

Reviewer Point 6: A table should be added for all parameters used.

→ **Authors:** Included.

Reviewer Point 7: Line 255: It is not clear to me why with small Phi the volume of the solid mantle has no effect on the time scale of chemical equilibration. Do the authors have an explanation? I think this also indicates that the material flow is extremely large - is this really realistic? One could estimate the value.

→ **Authors:** Coefficients of the fitting equation indicate that at low values of Φ, the ratio between volumes (i.e., the aspect ratio of the evolution scenario), has less impact than at high values of Φ. One possible explanation for this is that at low values of Φ, convection occurs with low degree, so the geometry of the problem is less important. We address this in the new version of the manuscript. Extremely large material flow is realistic, since $\Phi^+ \sim 10^{-5}$ and $\Phi^- \sim 10^{-3}$, according to Morison et al. (2019) and Morison (2019), for a purely thermal case.

Reviewer Point 8: Line 310: In the discussion, the crustal dichotomies of Mars and the Moon are mentioned and associated with the present process. I don't find this so obvious, because according to the model low degree convection is postulated at the beginning of the MO crystallization, but the crustal dichotomy is more likely to occur at the end of the MO phase, when the pattern becomes small scale.

→ **Authors:** We modified the text to address this point.

Reviewer Point 9: Line 370: It is stated that smaller planets cool faster. This is not generally true, for example if a blanketing crust is formed during MO crystallization before the mantle is entirely solid and the cooling and crystallization of the MO slows down considerably - as postulated for the Moon.

→ **Authors:** This is a good point and we modified the text to address it. Indeed it is not clear what could happen to smaller planets than Earth. In these smaller planets, Ra number is lower, which could imply that equilibration may take longer. However, it also depends on the timescale of crystallisation of the magma ocean. On one hand, smaller planets tend to cool faster, as they contain a smaller total reservoir of heat (and volatiles), but on the other hand, if a blanketing crust is formed before the mantle is entirely crystallised, then the magma ocean would take longer to cool.

Reviewer Point 10: Line 380: “for realistic values for the phase change number Phi+ smaller than $\sim$ 100”. I doubt that we really know the realistic value in view of the simplification of the process and the unknown parameters.

→ **Authors:** Indeed we don’t know an exact value of Φ. However, Morison et al. (2019) and Morison (2019) estimated $\Phi^+ \sim 10^{-5}$ and $\Phi^- \sim 10^{-3}$, for a purely thermal case. So small values of Φ are expected for the Earth. However, our paper includes a compositional treatment, and given that $\Phi^\pm$ is difficult to constrain, we vary this value between 10^{-1} and 10^5 (we use $\Phi^\pm = 10^{-1}$ as the lowest value possible for $\Phi^\pm$ because the resolution of the

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thermal boundary layer is computationally demanding once $\Phi^{\pm}$ decreases below 10^{-1}). In this paper we compare our estimated timescales for chemical (half-)equilibration with timescales of magma ocean crystallisation given by Lebrun et al., 2013. We see that for values of Φ lower that ~ 100, chemical (half-)equilibration occurs before magma ocean crystallisation (previous figure 8, now figure 7). Indeed the sentence “for realistic values for the phase change number Phi+ smaller than $\sim$ 100” might lead to confusion. What we meant is that low values of Φ are expected (Morison et al. (2019) and Morison (2019)), and we show that at any value below $\Phi^{\pm} \sim 100$, the system reaches chemical (half-)equilibration before magma ocean crystallisation. We changed this sentence to "Moreover, this efficient transfer of FeO renders the timescales of chemical (half-)equilibration between the solid mantle and magma ocean(s) shorter than (or on the order of) 1 Myr."

Reviewer Point 11: Figure 7 is difficult to read with the different symbols and lines.

→ **Authors:** We agree that figure 7 may be too complicated due to the amount of information. We remove figure 7 from this manuscript, since the main information is written in the text, and the good agreement of the scaling law with the predictions is made in figure A1.