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Solid Earth
Discussions

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

Anonymous Referee #1

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General comments

Bolrão *et al*. use the model of phase-change (permeable) dynamical boundary conditions (BCs) applied to a solid mantle bounded by a top magma ocean (TMO) and/or a basal magma ocean (BMO) to compute the timescale for chemical equilibration between these different reservoirs. The phase-change BCs, initially derived to describe the inner-core boundary, have been recently introduced in the context of magma oceans, and have been shown to possibly induce strong differences with cases considering classical free-slip BCs. This work takes a step forward in the task of constraining the effects of this dynamical setting in a realistic context. Specifically, it presents the

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first results of finite-amplitude thermo-chemical convection simulations using this type of BCs in a cylindrical geometry, using a spherical annulus mesh.

Depending on the "permeability" of the boundaries, quantified by the phase-change number (noted Φ), as well as the geometry of the problem (presence and thickness of a BMO and/or a TMO), the authors show that the convection pattern associated with the phase-change BCs (already presented in previous studies, e.g. Agrusta *et al.*, 2019) are recovered in this setting, and that they strongly influence the timing of chemical equilibration between the solid cumulates and the magma ocean(s). On the one hand, when the efficiency of phase-change at the boundary is low, mass transfer between the reservoirs is limited and chemical equilibration is portracted (or even never reached). On the other hand, when mass transfer is efficient at the boundarie(s), chemical equilibration is significantly sped up, and can be achieved on timescales shorter than those associated with magma ocean crystallization. The later case would rule out strong density heterogeneity in the solid cumulates induced by fractional crystallization of the magma ocean(s), and the resulting scenario of mantle overturn. The authors derive a scaling law to compute the characteristic time for equilibration as a function of Φ, the Rayleigh number, and the volume fraction of the already solidified mantle, that can be readily used by the community.

The article reads generally well, makes clear points and draws meaningful conclusions. I think that the description of the numerical setting and the fitting process should be elaborated, and the choice of figures adapted (see the specific comments). 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 twocomponent 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 $\alpha = 2 \times 10^{-5}\text{K}^{-1}$, ΔT=2000 K (typical value for the geometry used here with the melting curves from Fiquet *et al.*, 2010 for the initial temperature profile), $\rho_{\text{mantle}} = 4000$ kg/m^3 (as in Ballmer *et al.*, 2017) and B=1 (the value used in the present work), I found: $\Delta\rho = \alpha\Delta T B \rho_{\text{mantle}} = 160$ 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.

Specific comments

- 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?
- 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).
- 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).

- Please, include a table with the values of the different parameters and quantities used: h_{TMO}, h_S, h_{BMO} (and related R^+/R^- if relevant), Ra (and/or SC and Ra$_c$), B, $\Phi^\pm$, K, $X_{\mathrm{Fe}}^{\mathrm{bulk}}$.
- Line 86-87: "We ensure mechanical stability between the solid mantle and magma oceans, i.e., $\rho_{\mathrm{TMO}} < \rho_S < \rho_{\mathrm{BMO}}$". How do you do that? As far as I understand, density is only parametrized by X_{Fe}, and when you reach equilibrium, both TMO and BMO have the same X_{Fe} which should imply: $\rho_{\mathrm{TMO}} = \rho_{\mathrm{BMO}}$. 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.
- 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*.
- You assume that at equilibrium, X_{Fe} 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.
- 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?

- 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.

- The half-equilibrium time is parameterized using the parameters of the study: Ra, Φ and V_S/V_M. 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 X_{Fe}).

- 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.

- 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 H_2O and CO_2 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.

- 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.

- 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.

Technical corrections

- Line 26: "crystals start to appear and consolidate..."
- Line 42: ".. become denser with time." You could refer to Figure 1a where this process is represented.
- Line 58: As for Line 42, I would also refer to Figure 1b.
- Line 118: "is noted τ_η" rather than "is given by τ_η".
- 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".
- Line 172: "(similar to a half-life)" I would introduce the notion of half-equilibrium after calculating the equilibrium.
- Line 194: I think the correct word here is "bounded" (as you use it further).

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- Line 208: "... in dimensionless time units..."
- Line 210: "... thereby bringing the solid mantle and the TMO close to chemical equilibrium"
- 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 Φ=10-1 $\sim$10 times faster than for $\Phi = 10^2$, and $\sim$200 faster than for $\Phi = 10^3$).
- Line 214: "... for these three cases." or "... for these three values of Φ^-
- 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.
- Line 249: Shouldn't it be a minimum rather than a maximum?
- Caption Figure 6: "white circles" instead of "white colours".
- Table 1: It is not clear to me what the "error" is in this context.
- 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 a_3 to be close to 0, why is it not the case?
- Line 270: "Agrusta *et al*., 2019 showed"
- 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."

- Line 328-329: “Note that the thermal inertia of the core is similar to ...”

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