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<https://escholarship.org/uc/item/0xr6q6m7>

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Publication Date

2020-10-01

DOI

10.1016/j.epsl.2020.116502

Peer reviewed



Contents lists available at ScienceDirect

Earth and Planetary Science Letters

www.elsevier.com/locate/epsl


Reply to “Finding harzburgite in the mantle. A comment on Brown et al. (2020): ‘Markov chain Monte Carlo inversion of mantle temperature and source composition, with application to Reykjanes Peninsula, Iceland’” by Shorttle et al.

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ARTICLE INFO

Article history:

Accepted 25 July 2020

Available online xxxx

Editor: R. Dasgupta

Keywords:

mantle melting

Iceland

Markov chain Monte Carlo inversion

harzburgite

pyroxenite

1. Introduction

We welcome the opportunity to respond to Shorttle et al.'s (2020) comment on our paper, *Markov chain Monte Carlo inversion of mantle temperature and source composition, with application to Reykjanes Peninsula, Iceland*, recently published in *Earth and Planetary Science Letters* (Brown et al., 2020, v. 532, 116007). Shorttle et al.'s chief concern is that we did not include harzburgite in our published inverse models to reconcile geochemical and crustal thickness constraints for magmatism along the Reykjanes Peninsula. Here, we explain why our published models did not include or require harzburgite, and address the following specific points raised in their comment.

- The authors maintain that eqs. E1 and E2 presented in Appendix E of Brown et al. (2020), describing the proportion of pyroxenite-derived melt in the bulk igneous crust (X_{px}), are mathematically equivalent. These equations are only equivalent

when end-member melts are homogenized over a 2D melting zone. In our models, we assumed 1D homogenization of end-member melts. We elaborate on this point below.

- The authors claim that X_{px} predicted by our models (0.17–0.32) are nearly identical to those estimated by Shorttle et al. (2014) using natural lava compositions (0.3 ± 0.1) and, thus, our work adds no new insights into the contribution of pyroxenite-derived melt to the total melt at Iceland. Indeed, the values are similar, but the comparison is misleading as the value cited by Shorttle et al. (2020) pertains to magmatism in northeast Iceland, while our work focused on southwest Iceland (Reykjanes Peninsula), where Shorttle et al. (2014) reported higher mean X_{px} (0.4 ± 0.2). The comparison is also problematic for reasons alluded to above concerning assumptions about how end-member melts are homogenized.
- Finally, the authors assert that temperatures at the top of the melting zone predicted by our models are too low to agree with crystallization temperatures at Iceland, with the implication that had we included this constraint we would have required harzburgite in our models. We show below that temperatures predicted at the top of the melting zone in our models are indeed consistent with limited Al-in-olivine crystallization temperatures from the Reykjanes Peninsula (Spice et al., 2016).

DOI of original article: <https://doi.org/10.1016/j.epsl.2019.116007>.

DOI of comment: <https://doi.org/10.1016/j.epsl.2020.116503>.

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<https://doi.org/10.1016/j.epsl.2020.116502>

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2. Harzburgite or not?

In recent years great strides have been made in identifying refractory lithologies such as harzburgite in the convecting mantle, increasing our understanding of the significance and role of such lithologies for the evolution and dynamics of the Earth's interior (e.g., Stracke et al., 2019). A clear challenge in incorporating harzburgite in forward or inverse models of mantle melting that rely on the geochemistry of basalts is that it does not contribute much, if any, melt in the melting intervals for lherzolite and pyroxenite. Thus, in our inverse models we initially assumed a bi-lithologic source containing peridotite and pyroxenite, in part for simplicity, and because clear contributions of peridotite- and pyroxenite-derived melts have been identified at Iceland (Shorttle and MacLennan, 2011). For this bi-lithologic source (for which different varieties of pyroxenite were considered), the inversions reported in Brown et al. (2020) found combinations of potential temperature (T_P), pyroxenite abundance (Φ_{px}), and trace element and isotopic compositions of the peridotite and pyroxenite sources that matched the compositions of primitive end-member peridotite- and pyroxenite-derived melts, and the composition and thickness of the igneous crust. That is, the models reconciled the geochemical and geophysical observations without including harzburgite.

In light of the conclusions of Shorttle et al. (2014) and Matthews et al. (2016) that harzburgite is an important component of the Iceland source, we did run inversions that included (non-melting) harzburgite as a free parameter during the course of work for Brown et al. (2020). But, because we lacked additional constraints, such as plume volume flux (as imposed by Shorttle et al., 2014) or crystallization temperatures (as used by Matthews et al., 2016), for the Reykjanes Peninsula, our models including harzburgite only converged when T_P hit its upper bound (1570 °C) in the *prior probability distribution*. It was therefore not possible to ascribe significance to these inversion results. In retrospect, we should have noted this negative result, but submit that plume volume fluxes (see Jones et al., 2014, for a summary of estimates) are not sufficiently well-constrained at present to be of much value in our inversion approach. Likewise, crystallization temperatures, especially preferred temperatures recovered from the Al-in-olivine geothermometer, are scant for southwest Iceland (Spice et al., 2016) and thus are not a robust constraint, unlike the case for northeast Iceland (e.g., Matthews et al., 2016).

3. On the equivalency of eqs. E1 and E2 in Brown et al. (2020)

Equation E1 presented in Appendix E of Brown et al. (2020) is the relation used by Shorttle et al. (2014) to constrain the proportion of pyroxenite-derived melt in the bulk igneous crust (X_{px}) from natural lava compositions. Equation E2 is the relation we used in our forward melting calculation (REEBOX PRO; Brown and Leshner, 2016) to quantify X_{px} , and is not, as claimed by Shorttle et al. (2020), the equation employed by Shorttle et al. (2014) in their forward melting calculations that included the effects of compaction. In their comment, Shorttle et al. (2020) present a detailed derivation to argue that eqs. E1 and E2 are mathematically equivalent. However, these equations are mathematically equivalent only under the implicit assumption that end-member peridotite- and pyroxenite-derived melts are homogenized over their respective 2D melting zones. We argued (see sections 3.1 and 3.2.2, and Fig. 3 in Brown et al., 2020) that end-member melts for the Reykjanes Peninsula represent instantaneous melts homogenized along their respective 1D melting columns. In short, we could not compare estimates of X_{px} made using eq. E1 to X_{px} derived from our models (determined from eq. E2) because the key assumption made by Shorttle et al. (2014) and Matthews et al. (2016) of 2D homogenization was not met in our models. In Brown et al. (2020) we

therefore were not questioning the equivalency of eqs. E1 and E2 in the works of Shorttle et al. (2014) and Matthews et al. (2016), where the assumption of 2D homogenization holds. Rather, we were pointing out that eq. E1 does not provide an applicable constraint to our models that assumed 1D homogenization.

During our work leading to Brown et al. (2020) we also ran inversions assuming 2D homogenization of end-member melts for pyroxenite-bearing peridotite sources. However, we found that these models consistently returned heavy rare earth element (HREE) concentrations for the end-member peridotite-derived melt that were systematically too low to match the observations. As shown in Fig. 1, these HREE misfits remain even when including harzburgite. These misfits result from the larger contribution of low degree melts from the garnet stability field compared to models where 1D homogenization is assumed (see Fig. 1). While the manner in which instantaneous (fractional) melts accumulate in the melting zone beneath Iceland remains speculative, we find using our inversion approach we obtain the best fits to the observational constraints, at least for Reykjanes Peninsula, when end-member melts are homogenized over their 1D melting columns.

4. Dependence of X_{px} on the style of end-member melt homogenization

Comparison of the inversion results for 1D versus 2D homogenization provided in Fig. 1 illustrate another important aspect of the problem. By assuming 2D homogenization, 30% harzburgite and KG1 pyroxenite in the source, we find $X_{px} \sim 0.46$. This value is in good agreement with the mean X_{px} (0.4) determined by Shorttle et al. (2014) using primitive basalt compositions from southwest Iceland. However, assuming 1D homogenization, as done by Brown et al. (2020), X_{px} is ~ 0.26 for this harzburgite-bearing source – a proportion nearly identical to that reported in Brown et al. (2020) for a harzburgite-free source (0.22). This comparison highlights the dependence of X_{px} on the style of end-member melt homogenization, and the difficulty in directly comparing values of X_{px} that are implicitly or explicitly based on different styles of melt homogenization. It is also noteworthy that the choice of pyroxenite is important, and as shown in Fig. E1 of Brown et al. (2020), inversions using G2, KG1, and MIX1G pyroxenites matching the same geochemical and crustal thickness constraints yield X_{px} of ~ 0.32 , 0.22, and 0.17, respectively. In each case, X_{px} predicted by our models is less than the mean value estimated by Shorttle et al. (2014) for southwest Iceland. From these results, we maintain that matching melt compositions directly, as done by Brown et al. (2020), offers a robust estimate for X_{px} , whether one assumes 1D or 2D melt homogenization. We further contend that since we do not necessarily know *a priori* the style of melt homogenization, there is great value in having an approach that permits the style of end-member melt homogenization to be explored.

Lastly, Shorttle et al. (2020) claim that X_{px} in the models of Brown et al. (2020) are very similar to Shorttle et al.'s (2014) estimated value of 0.3 ± 0.1 , and thus place identical constraints on the contribution of pyroxenite to total melt production. This claim is misleading since they found X_{px} of 0.3 ± 0.1 , 0.6 ± 0.2 , and 0.4 ± 0.2 for northeast Iceland, central Iceland, and southwest Iceland, respectively, by applying eq. E1 to a large range of trace element pairs (see Fig. 3 in Shorttle et al., 2014). Thus, the claim that pyroxenite contributes $\sim 30 \pm 10\%$ to the total melt production at Iceland is strictly true only for northeast Iceland, which represents the lower end of the Iceland range found by Shorttle et al. The fact that we predict X_{px} for the Reykjanes Peninsula that is similar to northeast Iceland is perhaps fortuitous, but not meaningful, since comparison should be made with Shorttle et al.'s (2014) value for southwest Iceland (0.4 ± 0.2). Thus, it is clear to us that the assumptions built into our respective models have led us to different

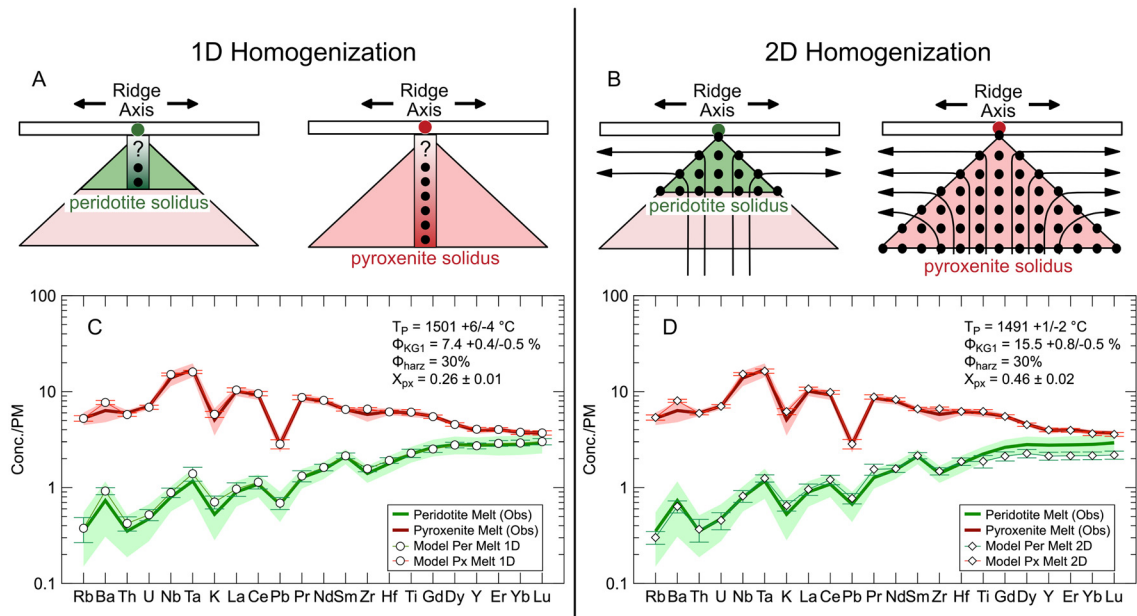


Fig. 1. 1D vs. 2D melt homogenization of end-member peridotite- and pyroxenite-derived melts. **A)** Schematic cross-section of melting zone showing 1D homogenization of instantaneous fractional melts (black dots) along longest melting columns for peridotite (left) and pyroxenite (right) sources. In the inversions of Brown et al. (2020) the proportion of the melting column over which these melts were accumulated was a free parameter, with all models showing accumulation of peridotite and pyroxenite-derived melts over nearly the entirety of their respective melting columns. **B)** Schematic cross-section of melting zone showing 2D homogenization of instantaneous melts (black dots) for peridotite (left) and pyroxenite (right) sources. **C)** Markov chain Monte Carlo inversion results for KG1 pyroxenite assuming 30% harzburgite (fixed). Primitive Mantle (McDonough and Sun, 1995)-normalized *posterior* peridotite- and pyroxenite-derived model melts (thin curves with open symbols and error bars showing 1 standard deviation) homogenized over their 1D melting columns are compared to the mean and standard deviation of end-member peridotite (thick green curve and green shaded field, respectively)- and pyroxenite (thick red curve and red shaded field, respectively)-derived melt compositions used in the *likelihood function* of Brown et al. (2020). **D)** Same as panel C except end-member model melts are homogenized over their respective 2D melting zones. Median and associated upper and lower quartile values for potential temperature, KG1 pyroxenite abundance, and the proportion of pyroxenite-derived melt comprising the bulk crust are given for the inversions shown in panels C and D. (For interpretation of the colors in the figure(s), the reader is referred to the web version of this article.)

conclusions regarding the contribution of pyroxenite-derived melts forming the crust in southwest Iceland. Reconciling these differences in time will be a mark of progress.

5. On the comparison of model and crystallization temperatures

Finally, Shorttle et al. (2020) claim that the temperatures at the top of the melting zones in the models presented by Brown et al. (2020) are too low to match crystallization temperatures at Iceland. Assuming the median T_p and Φ_{px} values for our G2, KG1, and MIX1G inversions, the temperatures at the tops of the respective melting zones in our models are $\sim 1329^\circ\text{C}$, $\sim 1337^\circ\text{C}$ and $\sim 1350^\circ\text{C}$, respectively. These values are *higher, not lower*, than the available Al-in-olivine crystallization temperatures ($\sim 1244\text{--}1316^\circ\text{C}$) derived from a single sample from Háleyjarbunga on the Reykjanes Peninsula (Spice et al., 2016). The olivine compositions in this lone sample are more evolved ($F_{0.89,8-89.9}$) than the most primitive olivines in this locale ($F_{0.91,1}$; Thomson and MacLennan, 2013), and thus likely record cooler temperatures than those of more primitive olivines that would better represent the temperatures at the top of the melting zone (e.g., Matthews et al., 2016). Thus, while data are limited for the Reykjanes Peninsula, available crystallization temperatures are broadly consistent with the temperatures at the top of the melting zone found in our models that did not include harzburgite. Therefore, harzburgite is not required to match this potential additional constraint for the Reykjanes Peninsula, as implied by Shorttle et al. (2020).

6. Final thoughts

We believe the inverse modeling method presented by Brown et al. (2020) offers a flexible tool allowing one to investigate many key assumptions required to relate basalt compositions and

volumes to the underlying physiochemical state of their mantle sources. Further, it is our view that new and robust insights into the Iceland source will come from complementary approaches that are continually refined as new data, insights into the melting processes, and numerical tools for interrogating these processes become available. The role of harzburgite is but one of the important outstanding questions about the constitution and properties of the convecting mantle.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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