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# Seismological evidence for thermo-chemical heterogeneity in Earth's continental mantle

Federico D. Munch<sup>1,\*</sup>, Amir Khan<sup>2,1</sup>, Benoit Tauzin<sup>3,4</sup>, Martin van Driel<sup>1</sup>,  
Domenico Giardini<sup>1</sup>

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## Abstract

Earth's thermo-chemical structure exerts a fundamental control on mantle convection, plate tectonics, and surface volcanism. There are indications that mantle convection occurs as an intermittent-stage process between layered and whole mantle convection in interaction with a compositional stratification at 660 km depth. However, the presence and possible role of any compositional layering in the mantle remains to be ascertained and understood. By interfacing inversion of a novel global seismic data set with petrologic phase equilibrium calculations, we show that a compositional boundary is not required to explain short- and long-period seismic data sensitive to the upper mantle and transition zone beneath stable continental regions; yet, radial enrichment in basaltic material reproduces part of the complexity present in the data recorded near subduction zones and volcanically active regions. Our findings further indicate that: 1) cratonic regions are characterized by low mantle potential temperatures and significant lateral variability in mantle composition; and 2) chemical equilibration seems more difficult to achieve beneath stable cratonic regions. These findings suggest that the lithologic integrity of the subducted basalt and harzburgite

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may be better preserved for geologically significant times underneath cratonic regions.

*Keywords:* Mantle thermo-chemistry, receiver functions, surface wave dispersion, petrologic phase equilibrium calculations

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## 1 1. Introduction

2 Since the recognition that plate tectonics is driven by solid-state mantle  
3 convection in the late 1960s, geoscientists have been debating mantle thermo-  
4 chemical structure and the detailed morphology of convection. Geochemical  
5 analysis of volcanic rocks (e.g., Pearson et al., 2003) support the existence of  
6 distinct reservoirs suggesting the mantle to be compositionally and dynami-  
7 cally layered, with the 660-km seismic discontinuity acting as compositional  
8 boundary. However, three-dimensional images of mantle structure from seismic  
9 tomography (e.g., French and Romanowicz, 2014; Schaeffer and Lebedev, 2013)  
10 indicate that subducted oceanic plates (known as slabs) can penetrate into the  
11 lower mantle as well as stagnate in the mantle transition zone (MTZ; region  
12 between 410 and 660 km depth) and around  $\sim 1000$  km depth, which rules out  
13 global layering at 660-km and appears to support whole-mantle convection in-  
14 stead. A range of hypotheses have been proposed to reconcile these observations  
15 (e.g., leaky layering at 660 km, layering deeper in the mantle, and ubiquitous  
16 compositional heterogeneity), yet the detailed morphology of convection pat-  
17 terns remains a matter of debate. The key question is whether the 660-km  
18 discontinuity is caused by a change in chemical composition (e.g., Anderson,  
19 2007) in addition to the endothermic ringwoodite $\rightarrow$ bridgmanite+ferropericlas  
20 phase transition (e.g., Ita and Stixrude, 1992).

21 Numerical modeling of subduction suggests that a lower-mantle enrichment  
22 in basalt ( $\sim 8\%$  with respect to the upper mantle) can explain slab stagnation  
23 at 660 and 1000 km depth, in the presence of whole-mantle convection (e.g.,  
24 Ballmer et al., 2015). This finding suggests that mantle convection occurs in an  
25 intermittent mode between layered- and whole-mantle convection, where slabs

26 penetrate intermittently in space and time, while a globally-averaged composi-  
27 tional stratification at 660 km depth is maintained (e.g., Tackley, 2000). Sup-  
28 porting evidence arises from direct comparison of one-dimensional Earth ref-  
29 erence velocity models and seismic observations sensitive to the bulk velocity  
30 structure of the mantle (P- and S-wave travel times and surface wave data)  
31 with estimates for a pyrolitic (Ringwood, 1975) and adiabatic mantle based on  
32 insights obtained from theoretical and experimental mineral physics. These  
33 studies report that pyrolitic and adiabatic mantle models cannot explain global  
34 observations (e.g., Cobden et al., 2008) and suggest that the lower mantle is ei-  
35 ther enriched (e.g., Murakami et al., 2012) or depleted (e.g., Khan et al., 2008)  
36 in silicon relative to the upper mantle. However, detailed analysis of SS and PP  
37 precursors that are sensitive to MTZ discontinuities, indicate that the observed  
38 amplitude variations (and even the absence of PP precursors in certain regions)  
39 are well-explained by lateral changes in mantle temperature or aluminium con-  
40 tent for a pyrolite mantle (Deuss et al., 2006).

41 Here, we investigate whether compositional mantle stratification is required  
42 to jointly explain seismic data sensitive to upper mantle and transition zone  
43 beneath a number of different tectonic settings by implementing a methodology  
44 that interfaces geophysical inversion of seismic data with self-consistent calcu-  
45 lations of mineral phase equilibria (Munch et al., 2018). The prediction of rock  
46 mineralogy and its elastic properties as a function of pressure, temperature, and  
47 bulk composition allows for self-consistent determination of depth and sharpness  
48 of the 410- and 660-km seismic discontinuities as well as upper mantle veloc-  
49 ities. This enables the joint analysis of P-to-s receiver functions and Rayleigh  
50 surface wave dispersion data to directly infer global lateral variations of man-  
51 tle temperature and composition. Until now, both data types have never been  
52 combined to resolve the structure down to the base of the MTZ.

## 53 **2. Materials and Methods**

### 54 *2.1. P-to-s receiver functions*

55 P-to-s receiver functions (hereinafter RF) are the records of compressional  
56 waves that convert into shear waves when encountering a discontinuity in mate-  
57 rial properties and are sensitive to sharp seismic discontinuities within a depth-  
58 dependent annulus underneath seismic stations (see Figure 1). Conversions  
59 occurring at the 410-km (P410s) and 660-km (P660s) discontinuities are rou-  
60 tinely used for detection of mineralogical phase changes at 410 and 660 km  
61 depth (e.g., Helffrich, 2000; Lawrence and Shearer, 2006b; Tauzin et al., 2008),  
62 but are rarely inverted to determine MTZ elastic structure (e.g., Schmandt,  
63 2012; Lawrence and Shearer, 2006a). Building on previous experience (Munch  
64 et al., 2018), we here invert RF waveforms to directly map global variations in  
65 mantle temperature and composition.

66 To this end, we first constructed a new global high-quality dataset of RF  
67 waveforms. The data consists of three-component seismograms recorded at 155  
68 broad-band permanent stations between 1997 and 2018. In order to ensure a  
69 good signal-to-noise ratio, only teleseismic events for epicentral distances be-  
70 tween  $40^\circ$  and  $95^\circ$  with magnitudes larger than 6 were selected. RF waveforms  
71 at each station were obtained by: 1) filtering of the records in the period range  
72 1–100 s; 2) rotation of the seismograms into radial, transverse, and vertical  
73 components; 3) calculation of signal-to-noise ratio between the maximum ampli-  
74 tude of the signal and the averaged root-mean-square of the vertical component;  
75 4) construction of RF waveforms through iterative time domain deconvolution  
76 (Ligorria and Ammon, 1999) for traces with signal-to-noise ratio larger than  
77 5; and 5) low-pass filtering of the RF waveforms to remove frequencies higher  
78 than 0.2 Hz. Finally, RF waveforms were corrected for move-out (using IASP91  
79 velocity model and a reference slowness of 6.5 s/deg) and subsequently stacked.  
80 Error on the stacked amplitudes were estimated using a bootstrap resampling  
81 approach (Efron and Tibshirani, 1991).

82 *2.2. Data selection*

83 The inversion of RFs requires careful waveform inspection to ensure high  
84 quality data. The stations were classified into three quality classes by visual  
85 inspection of the stacked RF waveforms (see Figure 2 and Table S1). Type-A  
86 stations correspond to RF waveforms with high signal-to-noise ratio and clear  
87 P410s and P660s signals. Type-B stations are characterized by RF waveforms  
88 with high signal-to-noise ratio but the signals corresponding to either the P410s  
89 or P660s conversions cannot be clearly isolated due to the potential presence  
90 of interfering seismic phases or complex three-dimensional structure. Type-C  
91 stations correspond to locations where only a small number of data could be  
92 stacked resulting in highly noisy RF waveforms with no clear P410s and P660s  
93 signals.

94 We found 48 stations for which the signals corresponding to either the P410s  
95 or P660s conversions cannot be unambiguously isolated (Type-B stations in  
96 Figure 2 and Figure S1). These stations are often located in regions where  
97 structure has previously been identified in seismic tomography models (e.g.,  
98 Schaeffer and Lebedev, 2013) such as subducted slabs in northeast Asia and the  
99 Mediterranean Sea. Our analysis focuses on 103 stations (Type-A stations in  
100 Figure 2) mainly located away from plate boundaries, where the RF waveforms  
101 can be accurately modeled with relatively low computational cost by methods  
102 that simulate full seismic wave propagation from source to receiver in spherical  
103 1D Earth models.

104 *2.3. Rayleigh wave dispersion data*

105 Rayleigh wave phase velocities are sensitive to the bulk velocity structure  
106 of the upper mantle and provide a better global coverage than the RFs, but  
107 with lower lateral resolution ( $\sim 650$  km). Here, we enhanced our RF data by  
108 extracting phase velocity dispersion curves for each station from the most recent  
109 available global data set of Rayleigh wave phase velocity dispersion (Durand  
110 et al., 2015). The data set consists of 60 phase velocity maps and uncertainties

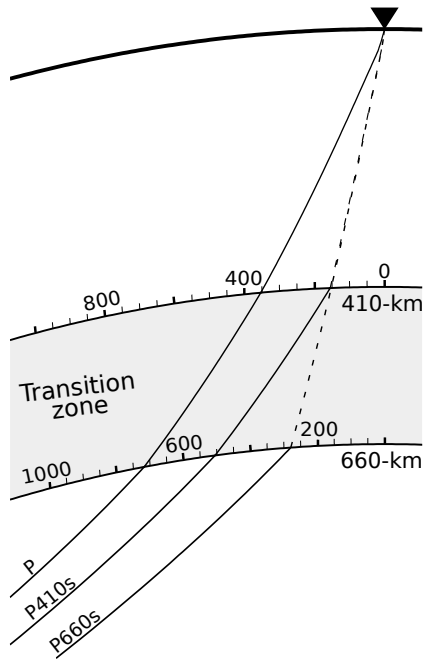


Figure 1: Schematic representation of teleseismic P-to-s waves scattered in the mantle transition zone and recorded at a seismic station (black triangle) located at an epicentral distance of  $40^\circ$ . Solid and dashed lines correspond to P and S ray path segments, respectively. The distance from the receiver along the 410-km and 660-km discontinuities is indicated in kilometers. The conversion points at 410-km and 660-km depth are laterally shifted from the station by  $\sim 150$  km and  $\sim 250$  km, respectively. Figure modified from Tazuin et al. (2008).

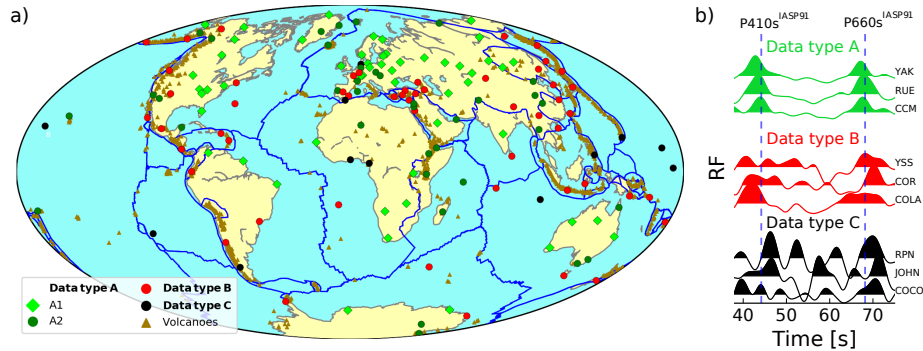


Figure 2: Geographic distribution of seismic stations. a) In all 155 seismic stations were considered and classified by data quality (type A, B, and C). Type A stations are subdivided into two further categories based on the data fit, labelled “A1” and “A2”. b) Examples of observed receiver functions (RF) for each data class.

111 covering the period range 40–250 s for the fundamental mode and up to the  
 112 fifth overtone on a  $2^\circ \times 2^\circ$  grid.

113 We would like to note that this data set is the result of a global tomographic  
 114 inversion and hence is affected by the chosen regularization. If overly damped,  
 115 phase velocity maps will be smoothed as a result of which dispersion curves  
 116 and RF waveforms might possibly sense slightly different structure.

#### 117 2.4. Model parameterization and forward problem

118 The crustal structure underneath each station is described in terms of a  
 119 set of layers with variable S-wave velocity  $V_s^i$  and thickness  $d^i$  ( $i = 1, \dots, 5$ ).  
 120 Mantle velocities below the Moho are derived from a set of model parameters  
 121 that describe mantle composition and thermal structure (Munch et al., 2018).  
 122 The former is parameterized in terms of a single variable (f) that represents  
 123 the amount of basalt in a basalt-harzburgite mixture, with the composition of  
 124 basalt and harzburgite end-members described using the CFMASNa chemical  
 125 model system comprising the oxides CaO-MgO-FeO-Al<sub>2</sub>O<sub>3</sub>-SiO<sub>2</sub>-Na<sub>2</sub>O. Mantle  
 126 thermal structure is delineated by a conductive lithosphere (linear gradient) on  
 127 top of an adiabatic geotherm. The lithospheric temperature is defined by the



128 temperature ( $T_0$ ) at the surface and the temperature ( $T_{\text{lit}}$ ) at the bottom of  
129 the lithosphere. The bottom of the lithosphere ( $z_{\text{lit}}$ ) corresponds to the depth  
130 at which the conductive lithospheric geotherm intersects the mantle adiabat  
131 defined by the entropy of the lithology at the temperature  $T_{\text{lit}}$  and pressure  $P_{\text{lit}}$ .  
132 This simplification allow us to treat continents as conducting lids that float atop  
133 the convecting mantle. The pressure profile is obtained by integrating the load  
134 from the surface.

135 Mantle mineralogy and its elastic properties as a function of depth are com-  
136 puted by means of free-energy minimization (Connolly, 2009; Stixrude and  
137 Lithgow-Bertelloni, 2011). Furthermore, shear attenuation is self-consistently  
138 derived from the shear modulus, temperature, and pressure profiles using the  
139 extended Burgers viscoelastic model (e.g., Bagheri et al., 2019). The resulting  
140 velocity and attenuation profiles are then used to compute synthetic RF wave-  
141 forms and Rayleigh wave phase velocities. The former are computed with the  
142 reflectivity method (Muller, 1985) replicating the slowness distribution recorded  
143 at each station and the same processing scheme applied on the observed seismo-  
144 grams. The latter are estimated using a spectral element-based python toolbox  
145 (Kemper et al., 2020; A spectral element normal mode code for the generation  
146 of synthetic seismograms; manuscript in preparation).

147 The choice of chemical model parameterization relies on its proximity to  
148 mantle dynamical processes, i.e., partial melting of mantle material along mid-  
149 ocean ridges. This process produces a basaltic crust and its depleted residue  
150 (harzburgite), which are cycled back into the mantle at subduction zones and  
151 become entrained in the mantle flow and remixed. In spite of its simplicity, the  
152 concept of distinct chemical end-member compositions has been found to pro-  
153 vide an adequate description of mantle chemistry, at least from a geophysical  
154 point of view (e.g., Xu et al., 2008; Khan et al., 2009; Ritsema et al., 2009).  
155 Furthermore, the use of the CFMASNa model chemical system allows us to  
156 account for the effect of transitions in the olivine, garnet, and pyroxene compo-  
157 nents of the mantle. As a consequence, and in contrast to usual seismological  
158 practice (e.g., Lawrence and Shearer, 2006b; Tauzin et al., 2008; Schmandt,

159 2012; Cottaar and Deuss, 2016), estimates of MTZ topography, volumetric ve-  
160 locities, and temperature derived here are independent of tomographic models  
161 or assumptions about the Clapeyron slope of pure  $(\text{Mg,Fe})_2\text{SiO}_4$ -phases.

162 The thermodynamic model presented here precludes consideration of redox  
163 effects (e.g., Cline II et al., 2018) as well as minor phases and components such  
164 as  $\text{H}_2\text{O}$  and melt due to lack of thermodynamic data. With regard to potential  
165 errors introduced by neglecting the effect of water, experimental evidence sug-  
166 gests that the presence of water would tend to thicken the transition zone by  
167 moving the olivine-wadsleyite transition up, while deepening the dissociation of  
168 ringwoodite (Frost and Dolejš, 2007; Ghosh et al., 2013). However, as discussed  
169 by Thio et al. (2015), it is currently not possible to quantify the effect of wa-  
170 ter on phase transitions because of the large uncertainties in thermodynamic  
171 data. In addition, the analyses performed by Thio et al. (2015) and Wang et al.  
172 (2018), where it is suggested that hydration of ringwoodite can significantly  
173 reduce elastic wave velocities, are based on experiments performed at ambient  
174 pressure conditions. A recent study by Schulze et al. (2018) showed that the  
175 hydration-induced reduction of seismic velocities almost vanishes at the tem-  
176 perature and pressure conditions of the transition zone. Density and elastic  
177 moduli are estimated to be accurate to within  $\sim 0.5\%$  and  $\sim 1\text{--}2\%$ , respectively  
178 (Connolly and Khan, 2016).

### 179 2.5. Inverse problem

180 The inverse problem is solved within a Bayesian framework where the so-  
181 lution is described in terms of the posterior probability distribution  $\sigma(\mathbf{m}|\mathbf{d}) \propto$   
182  $\rho(\mathbf{m})\mathcal{L}(\mathbf{m}|\mathbf{d})$ . The probability distribution  $\rho(\mathbf{m})$  describes the a priori informa-  
183 tion on model parameters (summarized in Table S2) and the likelihood function  
184  $\mathcal{L}(\mathbf{m}|\mathbf{d})$  represents a measure of the similarity between the observed data  $\mathbf{d}$  and  
185 the predictions from model  $\mathbf{m} = (T_{\text{lit}}, z_{\text{lit}}, f, V_s^1, \dots, V_s^5, d_1, \dots, d_5)$ . As time  
186 windows containing considerably small or no signal can introduce undesirable  
187 noise into the misfit function and unnecessarily increase the complexity of the  
188 misfit surface (Munch et al., 2018), the modeled and observed RF waveforms

189 are compared in three time windows defined by visual inspection of the ob-  
 190 served waveforms to include: 1) crustal signals ( $-5 \text{ s} < t < 30 \text{ s}$ ); 2) the P410s  
 191 conversion (generally observed in the time window 40 s–50 s); and 3) the P660s  
 192 conversion (typically recorded within the time window 60 s–80 s). Consequently,  
 193 the likelihood function can be written as

$$\mathcal{L}(\mathbf{m}|\mathbf{d}) \propto \exp \left\{ -\frac{1}{2} \sum_{i=1}^3 \phi_i^{\text{RF}}(\mathbf{m}|\mathbf{d}) - \frac{1}{2} \sum_{i=0}^5 \phi_i^{\text{SW}}(\mathbf{m}|\mathbf{d}) \right\}, \quad (1)$$

194 with

$$\phi_i^{\text{RF}}(\mathbf{m}|\mathbf{d}) = \frac{1}{3N_i} \sum_{j=1}^{N_i} \left[ \frac{\text{RF}^{\text{observed}}(t_j) - \text{RF}^{\text{modeled}}(\mathbf{m}, t_j)}{\delta \text{RF}^{\text{observed}}(t_j)} \right]^2 \quad (2)$$

195 and

$$\phi_i^{\text{SW}}(\mathbf{m}|\mathbf{d}) = \frac{1}{6M_i} \sum_{j=1}^{M_i} \left[ \frac{C_p^{i,\text{observed}}(T_j) - C_p^{i,\text{modeled}}(T_j, \mathbf{m})}{\delta C_p^{i,\text{observed}}(T_j)} \right]^2, \quad (3)$$

196 where  $C_p^i(T_j)$  denotes Rayleigh wave phase velocities for mode  $i$  and period  
 197  $T_j$  with  $M_i$  being the number of observed periods for each mode,  $\delta$  observed  
 198 uncertainties for each data type, and  $N_i$  the number of samples in each time  
 199 window of interest.

200 We sample the posterior distribution in the model space by combining a  
 201 Metropolis-Hastings Markov chain Monte Carlo (McMC) method (e.g., Mosegaard  
 202 and Tarantola, 1995) with a stochastic optimization technique (Hansen et al.,  
 203 2011). The latter is used to obtain a good initial model for the McMC algo-  
 204 rithm. This strategy improves the efficiency of the McMC method by signif-  
 205 icantly reducing the burn-in period. The McMC sampling is performed using  
 206 10 independent chains (with a total length of 10,000 iterations) characterized  
 207 by identical initial models but different randomly chosen initial perturbations.  
 208 This strategy allows for sampling 100,000 models with moderate computational  
 209 cost ( $\sim 3$  days using 10 cores). Finally, the 50,000 best-fitting candidates are  
 210 used to build histograms of the marginal probability distribution of each model  
 211 parameter.

### 212 **3. Results**

213 The seismic data are inverted using a Bayesian framework to provide es-  
214 timates of model range and uncertainty (see Sections 2.4 and 2.5). At each  
215 station, we recover marginal probability distributions of parameters describing  
216 crustal and mantle thermo-chemical structure (Figure 3b). By-products are as-  
217 sociated elastic profiles ( $V_p$ ,  $V_s$ , and density) for the upper mantle down to  
218 1000 km depth (Figure 3b). The sampled models must predict the observed  
219 Rayleigh wave phase velocities for the fundamental mode and overtones, as well  
220 as the main features of the observed RF waveforms (Figure 3a). Type-A sta-  
221 tions are further separated into two categories based on the quality of the data  
222 fit (Figure 2a) determined by visual inspection of the RF waveforms (Figure 3c  
223 and Figure S1) and Rayleigh wave dispersion curves (Figures S2–S3).

224 Our results suggest significant regional deviations from a compositionally  
225 uniform and adiabatic mantle. The retrieved models succeed in explaining the  
226 observed data in the inner part of continents (A1 stations in Figure 2a), but not  
227 near active plate boundaries such as in the western US or northeast Eurasia,  
228 in oceanic regions (Hawaii, Iceland, Samoa), or regions of intra-plate volcan-  
229 ism such as the Afar (A2 stations in Figure 2a). Among 93 stations in the  
230 continents, we succeed to fit the seismic data at 53 stations: 11 stations in  
231 Phanerozoic provinces of age younger than 600 Myr, 20 stations in 600-2000  
232 Myr old precambrian platforms, and 22 stations in cratonic regions older than  
233 2.2 Byr (Figure 4a).

234 We find mantle potential temperatures – equivalent to the temperature that  
235 the mantle would have at the surface, if it ascended along an adiabat with-  
236 out undergoing melting (McKenzie and Bickle, 1988) – ranging between 1450–  
237 1700 K (Figure 4b). These estimates are in good agreement with experimentally  
238 determined mantle potential temperatures ( $1610 \pm 35$  K) based on a pyrolitic  
239 composition (Katsura et al., 2010) and estimates derived from petrological and  
240 geochemical analysis of erupted lavas (1553–1673 K; Herzberg et al., 2007).  
241 Furthermore, we find that cratonic regions are characterized by low mantle po-

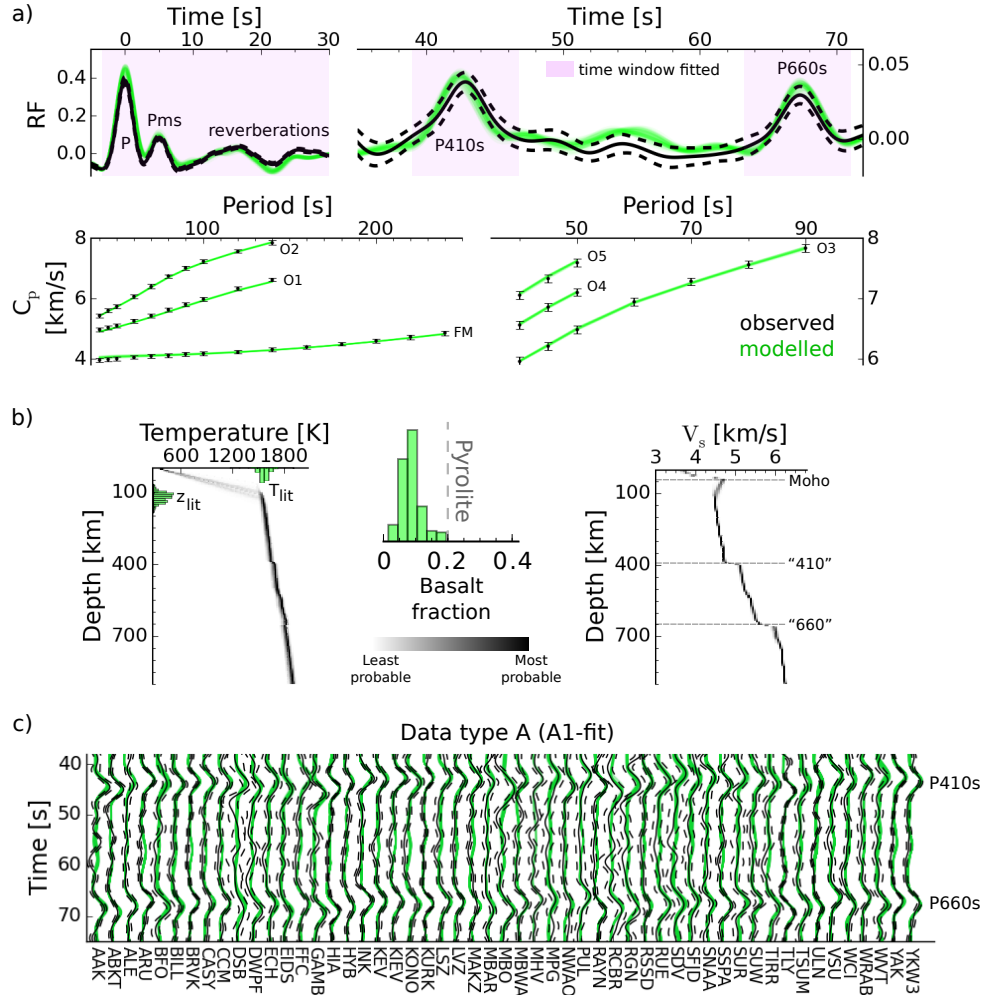


Figure 3: a) Example data fit (at station YAK) of RF waveforms and fundamental mode (FM) and overtone (O) Rayleigh wave phase velocities ( $C_p$ ). Observed data are shown in black and predictions in green. Magenta rectangles indicate the part of the RF waveform that is fitted in the inversion. b) Example inverted composition, thermal (temperature), and shear-wave velocity ( $V_s$ ) structure, including marginal posterior distributions of the main thermo-chemical parameters basalt fraction, lithospheric thickness ( $z_{lit}$ ) and temperature ( $T_{lit}$ ). c) Observed (black) and computed (green) RF waveforms for A1-fit stations (RF waveforms for A2-fit stations are shown in Figure S1).

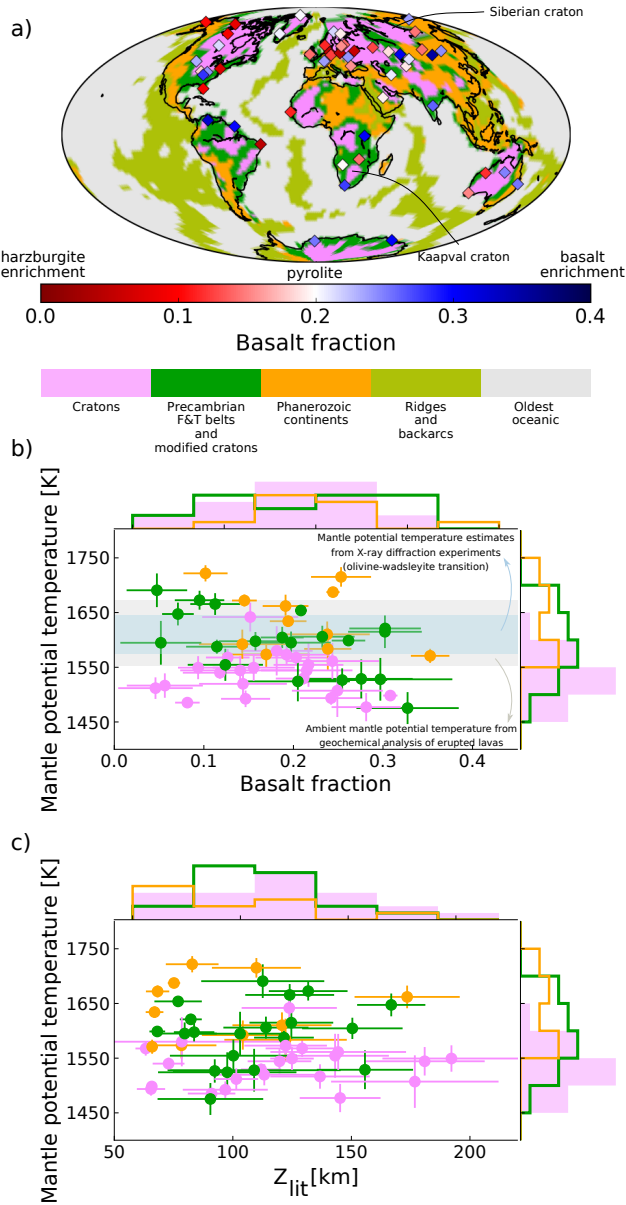


Figure 4: Global variations in mantle composition and thermal state. The results summarise the models that best fit (equivalent to the most probable model from the entire sampled model distribution) the observed data at each station and include both fully equilibrated as mechanically mixed models (see Figure 7). Panel a) depicts lateral variations in mantle composition (basalt fraction) for A1-fit stations (indicated by diamonds in Figure 2a). Coloured background shows a regionalised tectonic map derived from cluster analysis of tomographic models (Schaeffer and Lebedev, 2015). Panels b) and c) summarize most probable mantle potential temperature, basalt fraction, and thickness of the conductive layer ( $z_{lit}$ ) estimates classified by tectonic setting and shown as dots including error bars and along the axes as distributions. Coloured areas in panel b) depict experimentally-determined mantle potential temperatures for a pyrolitic composition (light blue, Katsura et al., 2010) and estimates derived from petrological and geochemical analysis of erupted lavas (yellow, Herzberg et al., 2007).

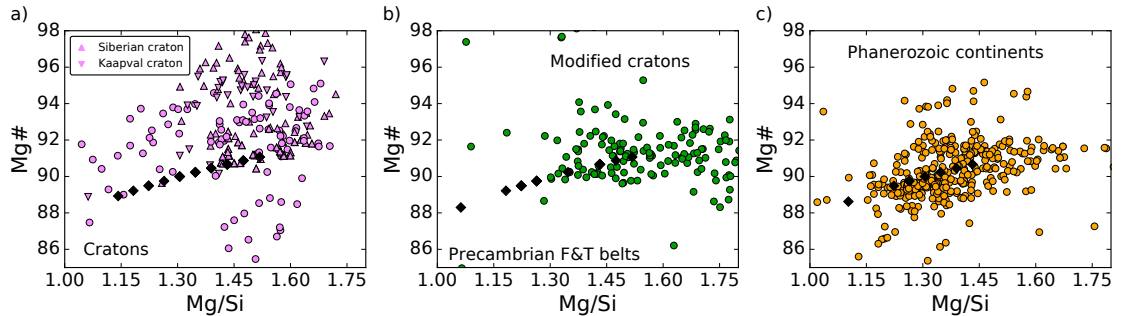


Figure 5: Variability in Mg# ( $\text{Mg}/(\text{Mg}+\text{Fe})$ ) and Mg/Si inferred in this study (black diamonds) and estimates derived from analysis of mantle xenoliths (coloured circles) extracted from the GEOROC database (<http://georoc.mpch-mainz.gwdg.de>) for different tectonic settings: a) cratonic regions; b) Precambrian fold-thrust belts; and c) Phanerozoic continents based on the tectonic regionalization of Schaeffer and Lebedev (2015).

242 tential temperatures (1450–1550 K) and significant lateral variability in mantle  
 243 composition ( $f \sim 0.05\text{--}0.30$ ), whereas higher mantle potential temperature esti-  
 244 mates (1600–1700 K) and smaller deviations from a pyrolitic mantle composition  
 245 ( $f \sim 0.1\text{--}0.25$ ) are recovered underneath Phanerozoic continents (see Figure 4b).  
 246 In addition, we find that Phanerozoic regions are characterized by relatively thin  
 247 thermal conductive layers (mean  $z_{\text{lit}} \sim 75$  km), whereas larger thicknesses (mean  
 248  $z_{\text{lit}} \sim 135$  km) are inferred underneath cratonic regions (Figure 4c).

249 The variability in mantle composition is in overall agreement with geo-  
 250 chemical observations that derive from analysis of mantle xenoliths – mantle  
 251 fragments carried to the surface by explosive eruptions – in the form of Mg#  
 252 ( $\text{Mg}/(\text{Mg}+\text{Fe})$ ) and Mg/Si estimates (see Figure 5), particularly for Precam-  
 253 brian fold-thrust belts (F&T belts) and Phanerozoic continents. Mantle xeno-  
 254 liths from Archean regions, in particular the Siberian and Kaapval cratons (indi-  
 255 cated in Figure 4a), are characterized by an excess in  $\text{SiO}_2$ . This Si-enrichment  
 256 was first believed to be a general characteristic of Archean subcontinental man-  
 257 tle (e.g., Boyd et al., 1997). However, lower  $\text{SiO}_2$  concentrations were measured  
 258 in xenoliths from the Slave (e.g., Kopylova and Russell, 2000) and North At-  
 259 lantic (e.g., Bernstein et al., 1998) cratons suggesting that Si-enrichment is a

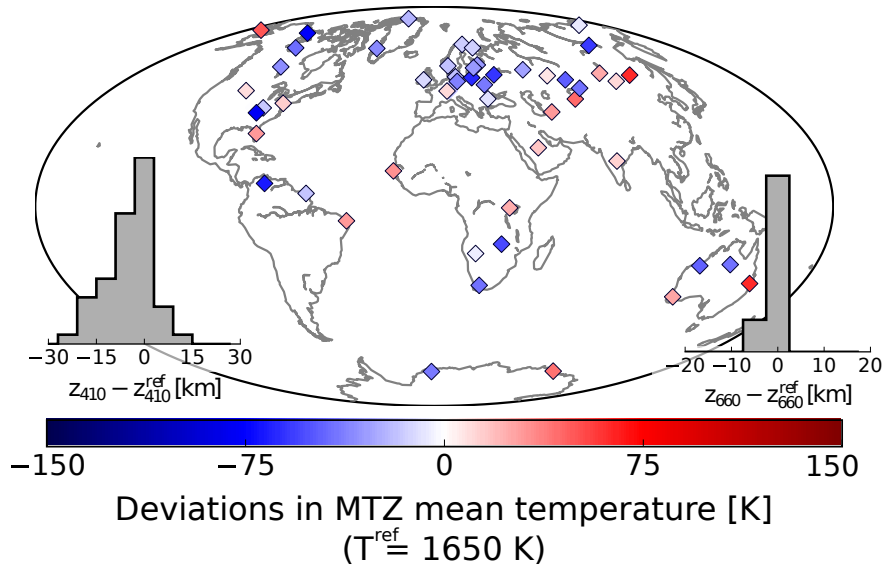


Figure 6: Relative lateral variations in mean mantle transition zone (MTZ) temperature and discontinuity topography (histograms). The latter show changes in the “410-” and “660-km” seismic discontinuities that bound the transition zone.

260 secondary (metasomatic) feature imposed upon the subcontinental mantle after  
 261 its formation as a residue of melting (Carlson et al., 2005). The compositional  
 262 changes imposed by such metasomatic processes can be addressed by extending  
 263 the chemical model to include other plausible end-members such as lherzolithic  
 264 and dunitic components.

265 In agreement with previous global studies (e.g., Deuss et al., 2013), we de-  
 266 termine an average MTZ thickness of  $\sim 250$  km with regional variations between  
 267 235 km and 270 km that mainly reflect changes in the topography of the 410-km  
 268 discontinuity (Figure 6). Furthermore, our results indicate that MTZ thickness  
 269 is linearly correlated with MTZ temperatures, whereas no clear correlation with  
 270 mantle composition can be identified (Figure S4). In addition, the recovered  
 271 crustal structure is in overall agreement with global crustal models (see Fig-  
 272 ure S5).

273 In order to test the robustness of the thermo-chemical variations reported  
 274 here, we performed two additional sets of inversions in which we fixed: 1) mantle



275 composition to pyrolite ( $f = 0.2$ ); and 2) mantle thermal parameters ( $T_{\text{lit}} =$   
276  $1623$  K and  $z_{\text{lit}} = 100$  km). We find that data are better explained ( $\sim 2$ – $15$   
277 % reduction in misfit values) when both thermal and compositional variations  
278 are considered (Figure S6). Furthermore, we find that it is not possible to  
279 explain the observed data solely by compositional variations (Figure S6c). This  
280 analysis confirms that although temperature plays a primary role in determining  
281 the seismic structure of the upper mantle and transition zone, the effect of  
282 composition cannot be neglected.

283 In addition, we investigated the correlation between the thermochemical param-  
284 eters inverted for here (Figure S7). As reported in previous work (Munch  
285 et al., 2018), no significant trade-offs are found between thermal and compo-  
286 sitional parameters signaling that temperature and composition are indepen-  
287 dently resolvable. In the context of erroneously mapping shallow into deeper  
288 structure, one could envisage mapping fast lithospheric phase velocities into cold  
289 temperatures. As a result, lower mantle temperatures would ensue, which corre-  
290 spond to larger MTZ thicknesses, and thus increased differential RF travel times.  
291 To compensate, a systematic decrease in basalt fraction would be required (see  
292 Figure 5 in Munch et al., 2018), which would result in a strong correlation be-  
293 tween mantle potential temperature and basalt fraction in the subcontinental  
294 mantle. Such a correlation is, however, not observed (see Figure 4b) indicat-  
295 ing that shallow cold continental structure is unlikely to be mapped into MTZ  
296 structure.

#### 297 **4. Discussion and implications**

298 Mineralogical models of the Earth typically view the mantle as either homo-  
299 geneous and pyrolitic (e.g., Ringwood, 1975) or chemically stratified with homo-  
300 geneous and equilibrated compositions in each layer (e.g., Mattern et al., 2005).  
301 To first order, such models are capable of explaining the observed composition of  
302 mid-ocean ridge basalts (e.g., McKenzie and Bickle, 1988) and seismic velocities  
303 of the upper mantle and transition zone (e.g., Ita and Stixrude, 1992). How-

304 ever, experimental measurements of mantle mineral chemical diffusivity (e.g.,  
305 Hofmann and Hart, 1978) suggest that equilibration may not be accomplished  
306 over the age of the Earth for the amount of stretching and folding predicted  
307 in mantle convection simulations (e.g., Nakagawa and Buffett, 2005). Further-  
308 more, trace element chemistry of basalts (Sobolev et al., 2007) also point to the  
309 mantle as consisting of a non-equilibrated mechanical mixture. This led to the  
310 concept of two distinct mantle compositional models (Xu et al., 2008): mechan-  
311 ical mixture and equilibrium assemblage. The former represents the scenario in  
312 which pyrolytic mantle has undergone complete differentiation to basaltic and  
313 harzburgitic rocks, whereas the latter assumes the mantle to be well-mixed and  
314 fully-equilibrated. These two types of mantle compositional models generate  
315 subtle differences that are rarely accounted for in the interpretation of seismic  
316 data (e.g., Ritsema et al., 2009).

317 Here, we have investigated the extent to which the mantle is well-mixed  
318 or chemically equilibrated by quantitatively comparing the quality of the data  
319 fit obtained for each compositional model. We find 42 stations for which rel-  
320 ative differences in the misfit values for the best-fitting models (calculated as  
321 described in Section 2.5) are larger than 5% (Figure S8). Our results suggest  
322 that the mantle is neither completely equilibrated nor fully mechanically mixed,  
323 but appears to be best described by an amalgam between the two with cratonic  
324 regions best characterized by a mechanically mixed model and Precambrian  
325 fold-thrust belts best described by an equilibrium assemblage (see Figure 7a).  
326 This suggests that the lithologic integrity of the subducted basalt and harzbur-  
327 gite is better preserved for geologically significant times beneath stable cratonic  
328 regions, i.e., chemical equilibration is more difficult to achieve. Further to this,  
329 the presence of lower potential mantle temperatures underneath cratonic regions  
330 support the existence of deep low-temperature continental roots whose signal  
331 extends into the MTZ (e.g., Jordan, 1978) and which might be isolated from  
332 the main mantle flow associated with ridges and trenches. In contrast hereto,  
333 our results suggest that these regions are not systematically depleted in basalt  
334 component.

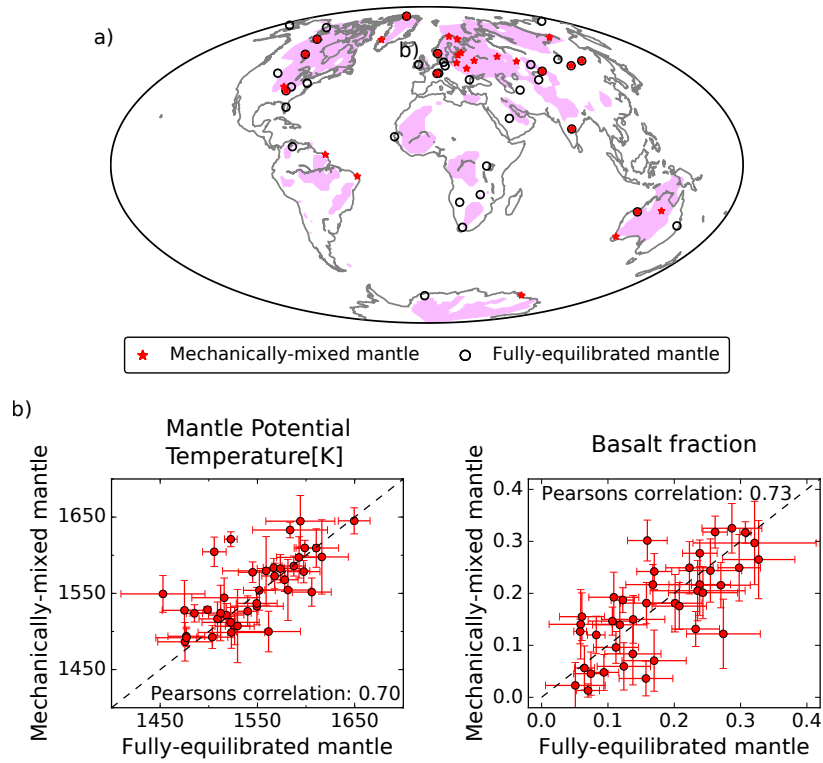


Figure 7: a) Global map of cratonic regions (pink areas) and distribution of stations for which the observed data are best explained by either a mechanically mixed or a fully equilibrated mantle compositional model. b) Most probable mantle potential temperature and basalt fraction estimates (shown as dots including error bars) retrieved for fully-equilibrated and mechanically-mixed mantle models.

335 Despite subtle differences, we find that temperature and compositional es-  
336 timates appear to be independent of compositional model (Figure 7b). This  
337 contrasts with a previous study (Ritsema et al., 2009) where the equilibrium as-  
338 semblage model was found to result in higher temperature estimates relative to  
339 the mechanical mixture model based on comparison of theoretical and observed  
340 differential travel times of waves reflected underneath the MTZ discontinuities.  
341 This discrepancy can be explained by the fact that Ritsema et al. (2009) 1) only  
342 considered a pyrolitic mantle composition and therefore mapped all variations  
343 of chemistry into temperature and 2) focused on regions of the mantle charac-  
344 terized by higher mantle potential temperatures ( $>1700$  K) for which differences  
345 in differential travel times predicted for distinct mantle compositional models  
346 are observed to be larger (cf. Figure 5 in Munch et al., 2018).

347 Laboratory experiments and numerical simulations of mantle convection sug-  
348 gest that continents can have a strong influence on mantle dynamics and the  
349 heat flow escaping from the Earth’s surface (e.g., Lenardic et al., 2011). In  
350 this context, it has been proposed that continents can act as thermal insula-  
351 tors by inhibiting heat loss, thereby increasing mantle temperatures regionally  
352 (e.g., Ballard and Pollack, 1987; Lenardic et al., 2005). For instance, Rolf et al.  
353 (2012) predicted a temperature increase of  $\sim 140$  K underneath continental re-  
354 gions relative to the sub-oceanic mantle, based on internally heated 3-D mantle  
355 convection simulations with various continental configurations. However, the  
356 influence of the insulating effect of continents on present-day mantle thermal  
357 state remains uncertain (cf, Jain et al., 2019). The mantle potential tempera-  
358 tures derived here (summarized in Figure 4b) suggest that the insulating effect  
359 might not be as prominent as predicted in mantle convection simulations.

360 A recent analysis of short-scale ( $\sim 10$  km) variations in 660-km discontinu-  
361 ity topography (Wu et al., 2019) suggested the potential existence of chemical  
362 layering at the top of the lower mantle. In this context, our results indicate  
363 that a compositional boundary at 660 km depth is not required beneath stable  
364 continental regions to explain the observed seismic signals. However, we find  
365 significant complexity in the RF waveforms (see Figure S1) recorded near ac-

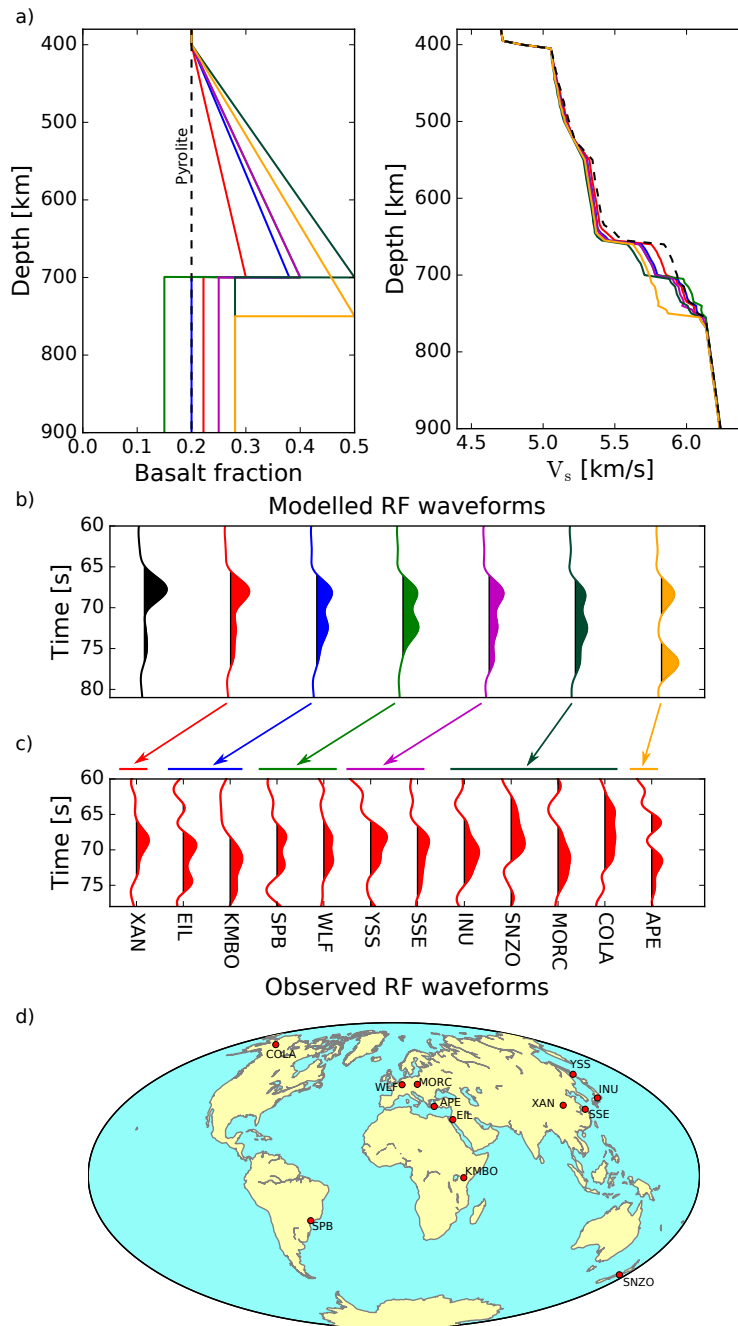


Figure 8: Comparison between observed and synthetic receiver function (RF) waveforms computed for different compositional gradients as predicted by mantle convection simulations (e.g., Ballmer et al., 2015). a) Compositional profiles and corresponding shear-wave velocity ( $V_s$ ) structures. b) Synthetic RF waveforms for each proposed model. c) Observed RF waveforms. d) Geographic location of stations considered in panel c.

366 tive plate boundaries (e.g., western US or northeast Eurasia), in oceanic regions  
367 (e.g., Hawaii and Iceland), and regions of intra-plate volcanism (e.g., Afar) that  
368 cannot be explained by a compositionally uniform and adiabatic mantle. Fig-  
369 ure 8 depicts synthetic RF waveforms computed for different depth-dependent  
370 compositional profiles based on predictions from mantle convection simulations  
371 (e.g., Tackley, 2008; Ballmer et al., 2015). We find an overall agreement between  
372 the observed and synthetic waveforms between 60 and 75 seconds (P660s) sug-  
373 gesting that a significant part of the complexity present in the RF waveform data  
374 between 60 and 75 seconds (P660s) can be explained by local radial changes in  
375 mantle composition. Variations in P660s travel time present in the observed RF  
376 waveforms (Figure 8c) most likely reflect local changes in upper mantle veloc-  
377 ities due to thermal and compositional variations. Despite being a qualitative  
378 comparison, this result supports the existence of local lower-mantle enrichment  
379 in basalt ( $\sim 5\text{--}10\%$  with respect to the upper mantle) and the local accumu-  
380 lation of basalt ( $\sim 15\text{--}30\%$ ) in the MTZ. A detailed characterization of these  
381 radial changes would require the use of more advanced wave propagation tech-  
382 niques (Monteiller et al., 2012) that account for effects introduced by complex  
383 three-dimensional structure. Compositional layering has also been found neces-  
384 sary to explain regional SS precursors signals beneath Hawaii (Yu et al., 2018)  
385 and narrow high-velocity anomalies beneath the MTZ in regions of mantle up-  
386 wellings (Maguire et al., 2017). Although the detailed morphology of mantle  
387 compositional gradients remains uncertain, all these observations support geo-  
388 dynamical simulations that describe mantle convection as a mixture of layered  
389 and whole-mantle convection (Tackley, 2000), where cold and/or basaltic ma-  
390 terial accumulates above 660 km depth until huge avalanches precipitate it into  
391 the lower mantle, “flushing” the local upper mantle through broad cylindrical  
392 downwellings to the core-mantle boundary in a globally asynchronous manner  
393 (e.g., Tackley, 2008).

## 394 5. Conclusions

395 In this paper, we investigated whether compositional mantle stratification  
396 is required to jointly explain short- (P-to-s receiver functions) and long-period  
397 (Rayleigh wave dispersion) seismic data sensitive to upper mantle and transition  
398 zone structure beneath a number of different tectonic settings. This is achieved  
399 by implementing a methodology that interfaces the geophysical inversion with  
400 self-consistent calculations of mineral phase equilibria on a new global high-  
401 quality dataset of receiver function waveforms from an initial pool of 155 stations  
402 enhanced with the most recent available global dataset of Rayleigh wave phase  
403 velocity dispersion for the fundamental mode and up to fifth overtone.

404 We showed that a compositional boundary is not required to explain short-  
405 and long-period seismic data sensitive to the upper mantle and transition zone  
406 beneath stable continental regions; yet, radial enrichment in basaltic material  
407 reproduces part of the complexity present in the data recorded near subduc-  
408 tion zones and volcanically active regions. Our findings further suggest that  
409 the mantle is neither completely chemically equilibrated nor fully mechanically  
410 mixed, but appears to be best described as an in-between amalgam. In particu-  
411 lar, chemical equilibration seems less prevalent beneath cratons suggesting that  
412 these regions are possibly isolated from convection processes.

413 Future work will focus on further investigation of the morphology of mantle  
414 compositional gradients near subduction zones and volcanically active regions.  
415 This will require the incorporation of: 1) a depth-dependent composition and  
416 deviations from adiabatic profiles; 2) wave propagation simulations based on  
417 more advanced waveform modeling (e.g., Monteiller et al., 2012) to account for  
418 three-dimensional effects; and 3) additional information from other geophysical  
419 techniques such as Love phase and group velocities (e.g., Khan et al., 2009; Calò  
420 et al., 2016) or S-to-p converted waves (Oreshin et al., 2008; Yuan et al., 2006)  
421 to improve the resolution in the upper mantle.

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