

Supplementary Information

In the transition-zone water-filter hypothesis, (see main text), water is assumed essentially trapped within the transition zone because of dehydration melting of ambient upwelling at 410km and exsolution of water from slabs at 660km. The assumption that recycling of water is closed allows us to develop a simple theoretical model with which to predict various important parameters such as the melt fraction of partially melted ambient upwelling (which determines how well incompatible elements are filtered out) and the average thickness of the melt layer. The model system is driven by a background circulation through the transition zone consisting of downwelling slabs and the resultant passive ambient upwelling. Super-saturation and melting occurs in ambient upwelling mantle after passing out of the transition zone. The resulting layer of heavy melt can reach a steady state in terms of its chemistry and thickness if all materials in the melt layer are removed by slab entrainment at the same rate they are injected by upwelling ambient mantle. Self-regulation of melt-layer growth (and thus a steady state) is attainable because the efficiency of slab entrainment increases as the melt-layer thickness (and hence the effective contact area between the slab and melt) increases. Here we examine the conditions for this steady state and predict the typical melt fraction of upwelling mantle, the melt-layer thickness, and chemistry (concentration of water and incompatible elements) of the transition zone and melt layer.

1 Background mantle circulation through the transition zone

The system is driven by an imposed background circulation prescribed by a downwelling slab flux and the resulting passive upwelling (assuming that the plume flux contribution is negligible). This circulation is prescribed by mass conservation, which requires that upwelling and downwelling mass fluxes across the 410km boundary balance; this leads to $2\pi R d_{slab} w_{slab} \approx 4\pi R^2 w_0$ where $R \approx 6000\text{km}$ is the radius of the 410km boundary, $d_{slab} \approx 100\text{km}$ is a typical slab thickness, $w_{slab} = 10\text{cm/yr}$ is an order-of-magnitude slab

descent velocity, and w_0 is the average ascent velocity of ambient upwelling mantle; we have assumed that the density of upwelling and downwelling currents are approximately the same and that the net length of the intersection of all slabs with the 410km boundary is approximately $2\pi R$ since most slabs occur in a nearly great circle around the Pacific rim (and any additional slabs largely compensate for the Pacific-rim being slightly smaller than a great circle). As also noted in the main text, this leads to an order of magnitude estimate of $w_0 \approx 1\text{mm/yr}$.

2 Melting of ambient upwelling mantle

Since ambient upwelling mantle leaving the transition zone is water super-saturated, it undergoes eutectic melting with a melt mass fraction (melt mass to total mass) of approximately

$$f = (X_a - X_{ol}^*)/X_m \quad (\text{S-1})$$

where X_a is the water mass fraction of ambient mantle rising out of the transition zone, X_{ol}^* is the water mass fraction of the solid-phase remaining after partial melting (denoted by its primary mineral, olivine) and X_m is the water mass fraction for the melt-phase. (Normally, the denominator of the right side of (S-1) is $X_m - X_{ol}^*$, however $X_m \gg X_{ol}^*$.) The relation (S-1) is valid for both binary and ternary eutectics as long as X_{ol}^* is small; here, for simplicity, we assume a binary system (silicate and water) since use of a ternary system does not change the essential results. In terms of aqueous chemical equilibrium, melting is likely closer to batch than fractional since ambient upwelling mantle moves very slowly and water (or hydrogen) diffusion is relatively fast (with diffusivity of at least $10^{-8}\text{m}^2/\text{s}$); moreover, since melt is assumed dense (see below) it stays trapped above the 410km boundary and thus retains greater contact with the slowly ascending solid matrix. In this case X_m is simply the liquidus water fraction at ambient mantle temperatures of 1800K, which is of order 10wt% (ref. 1). Finally, we assume X_{ol}^* is of order 0.1wt% (we use a number that is closer to the olivine solubility limit than to the considerably smaller

solidus water concentration, since this yields a more conservative estimate for melting).

3 Silicate and water fluxes in the melt layer

The upward mass flux of melt through the 410km boundary is approximately $f\rho_s w_0 4\pi R^2$ where ρ_s is silicate density (since the water mass fraction of the transition zone is a few percent or less). We assume a slab crossing the melt layer entrains silicates by cooling and solidification over zones on either side of the slab whose effective thicknesses, upon reaching the base of the melt layer, are δ_s (an average value since one side of the slab is probably cooler than the other). The mass flux balance of silicates in the melt is thus

$$(1 - X_m)f\rho_s w_0 4\pi R^2 = \rho_s w_{slab} \delta_s 4\pi R \quad (\text{S-2})$$

Slabs also entrain water through water-saturated silicates crystallizing onto or near the slabs and from diffusion of water into the slabs. Since slabs are cold and the melt is just above the olivine-wadsleyite boundary, the crystallizing silicates are in the wadsleyite phase and the relevant water-saturation value is that of wadsleyite at slab temperatures $X_{wd}^* = 3\text{wt}\%$ (see main text, Methods 3). Diffusion of water into the slab causes the water concentration to go from $X_s^0 = \chi X_{wd}^*$ (where $0 < \chi < 1$) at the slab-melt interface to approximately 0 over a diffusive boundary layer which at the base of the melt layer is $2\delta_w$ where

$$\delta_w = \sqrt{D_w h / w_{slab}} \quad (\text{S-3})$$

in which D_w is water (or hydrogen) diffusivity in solid wadsleyite and h is the thickness of the melt layer. The water mass flux balance is therefore approximately

$$X_m f \rho_s w_0 4\pi R^2 = \rho_s w_{slab} 4\pi R X_{wd}^* \left(\delta_s + \chi \int_0^{2\delta_w} \left(1 - \frac{y}{2\delta_w}\right) dy \right) \quad (\text{S-4})$$

Using (S-1), the silicate and water flux-balance equations become,

$$\frac{1 - X_m}{X_m} (X_a - X_{ol}^*) w_0 R = w_{slab} \delta_s \quad (\text{S-5})$$

$$(X_a - X_{ol}^*) w_0 R = X_{wd}^* w_{slab} (\delta_s + \chi \delta_w) \quad (\text{S-6})$$

respectively. These equations, however, are not sufficient since χ is unknown and both δ_s and δ_w depend on melt layer thickness h , which in turn depends on the water fractions X_m and X_a . In particular, since water is assumed trapped in the transition zone-melt layer system (see text) then the total mass of water in the system remains approximately fixed (assuming that the small amount of water carried out of the system by the solid-phase portion of the ambient upwelling as well as from plumes is essentially replenished by water transported from the surface by slabs), i.e.,

$$4\pi R^2(\rho_m X_m h + \rho_s X_a H) = 4\pi R^2 \rho_s X_0 H \quad (\text{S-7})$$

where H is the transition zone thickness, X_0 is the initial transition zone water concentration (i.e., without the melt layer) and ρ_m is the density of melt. Since the melt can have a significant water fraction, its density depends on X_m ; roughly assuming the melt is an effective mixture of liquid silicate with density $\sim \rho_s$ and water of density ρ_w then $X_m \rho_m = \theta \rho_w$ and $(1 - X_m) \rho_m = (1 - \theta) \rho_s$ where θ is the water volume fraction in the mixture; therefore, by eliminating θ , one obtains

$$\rho_m = \rho_s / (1 + \gamma X_m) \quad \text{where} \quad \gamma = \rho_s / \rho_w - 1 . \quad (\text{S-8})$$

The actual melt density is higher than this because of the dissolution of water in the melt (see Methods 2 of the paper); however, the above relation gives a first-order approximation with the proper limits at $X_m = 0$ and 1. The melt layer thickness is therefore

$$h = H(X_0 - X_a)(1 + \gamma X_m) / X_m \quad (\text{S-9})$$

4 Silicate entrainment zone

The solidification entrainment zone with maximum effective width δ_s involves freezing of the melt in the vicinity of the slab. At their interface, the melt and slab must be in local chemical equilibrium, i.e.,

$$\frac{X_m^0}{X_m^*} = \frac{X_s^0}{X_{wd}^*} = \chi \quad (\text{S-10})$$

where X_m^0 is the water concentration in melt adjacent to the slab and X_m^* is the water-saturation limit of melt, which is effectively 100wt% since silicate melt and water are extremely miscible at the pressures and temperatures near 410km depth². This simply implies that $X_m^0 \approx \chi$. The silicate entrainment zone is thus the solid fraction of the melt region adjacent to the slab that is cooled below the eutectic point and thus freezes. (The water concentration of the near-slab melt is much higher than what can be absorbed by solidifying crystals, and thus after freezing some water remains to be mixed with the new incoming melt; thus the wet melt undergoes only partial solidification in the freezing zone, which is why δ_s is referred to as an “effective width” since it is the width of the solidification zone as if it were compacted to a pure solid.) Near the base of the melt layer, the solidification zone has an effective mass (per unit area parallel to the slab-melt interface) of

$$\rho_s \delta_s = (1 - \chi) \rho_m^0 \delta_T \quad (\text{S-11})$$

where $\rho_m^0 = \rho_s / (1 + \gamma\chi)$ is the density of melt near the slab, and δ_T is the maximum width of the zone cooled below the eutectic temperature. Cooling of melt is controlled by convective heat transport from the melt into the slab via vertical-plate (or “window-pane”) convection. The maximum resistance to convective flow occurs where flow is percolative through the partial solidification zone, and thus we assume this is the rate-limiting drag region. We can estimate the convective heatflux into the slab by a basic scaling analysis³. Temperature T in the melt changes from T_1 by the slab to T_0 far from the slab, and thus we can write $T = T_0 + \Delta T \Theta$ where $\Delta T = T_1 - T_0$ and Θ is a dimensionless function varying between 0 and 1. Variations in temperature with distance y from the slab occurs over the cold convective thermal boundary layer sinking along the slab, which has a typical length scale of $L_c = \sqrt{\kappa h / W}$ where κ is thermal diffusivity. The convective velocity scale W is determined by the balance between thermal buoyancy and Darcy drag; thus $W = g\alpha\Delta T K_0 \phi^{n-1} / \nu$ where α is thermal expansivity, ν is the melt kinematic viscosity, K_0 is a reference permeability, ϕ is the porosity of the solidification zone, and n is a dimensionless number typically between 2 and 3 (see ref. 4). Therefore we express y in terms of the

horizontal scale of the system, i.e., $y = L_c \zeta = \frac{h}{\sqrt{R_p}} \zeta$ where ζ is dimensionless distance and $R_p = g\alpha\Delta T K_0 \phi h / (\kappa\nu)$ is the percolative Rayleigh number in which we have assumed for simplicity that $n = 2$. The average heatflow out of the melt into the slab is $\bar{q} = -\frac{k}{h} \int_0^h \frac{\partial T}{\partial y} dz$ at the slab-melt interface $y = 0$, where k is thermal conductivity; with our temperature and length scales, this leads to

$$\bar{q} = b \frac{k\Delta T}{h} \sqrt{R_p} \quad (\text{S-12})$$

where $b = -\frac{1}{h} \int_0^h \frac{\partial \Theta}{\partial \zeta} |_{y=0} dz$ is a dimensionless number necessarily of order 1 (since Θ goes approximately from 1 to 0 as ζ goes from 0 to 1; see also Bird et al.³).

The porosity of the partial solidification zone ϕ is given by eutectic crystallization whereby a unit volume of the zone has water mass $\rho_m^0 \chi = \phi \rho_w + \rho_{ss}(1 - \phi) X_{wd}^*$ and silicate mass $\rho_m^0 (1 - \chi) = \rho_{ss}(1 - \phi)(1 - X_{wd}^*)$ where ρ_{ss} is the density of a solid-solution silicate saturated with water; this leads to the relation

$$\phi = \left(\frac{1 + \gamma}{1 + \gamma\chi} \right) \left(\frac{\chi - X_{wd}^*}{1 - X_{wd}^*} \right) \quad (\text{S-13})$$

The local width of the zone that is cooled by the slab beneath the eutectic temperature is δ'_T which goes from 0 at the top of the melt layer $z = h$ to its maximum value δ_T at the base of the melt layer $z = 0$. The energy (per unit area parallel to the slab) extracted as this zone thickens from $\delta'_T(z)$ to $\delta'_T(z - dz)$ while the slab descends a distance dz is given by

$$-\rho_m^0 c_p b^* \Delta T \frac{d\delta'_T}{dz} dz = q \frac{dz}{w_{slab}} \quad (\text{S-14})$$

where c_p is heat capacity, and q is the local value of heatflow into the slab (such that its vertical average is \bar{q}); b^* is a dimensionless number to account for the fact that the melt need not be cooled by the full ΔT to undergo eutectic solidification, but that latent heat of fusion must also be removed; these are more or less offsetting effects and thus b^* is assumed of order 1. Integrating (S-14), applying the boundary conditions that $\delta'_T = 0$ at $z = h$ and $\delta'_T = \delta_T$ at $z = 0$, and employing (S-12) leads to

$$\delta_T = \frac{h\bar{q}}{b^* \rho_m^0 c_p \Delta T w_{slab}} = \frac{\kappa}{w_{slab}} \sqrt{R_p} \quad (\text{S-15})$$

where $\kappa = k/(\rho_m^0 c_p)$ and we assume b/b^* is of order unity.

Finally, using (S-11), (S-13) and (S-15), the solidification zone at the base of the melt layer is

$$\delta_s = \sqrt{L_s \Gamma(\chi) h} \quad (\text{S-16})$$

where

$$\Gamma(\chi) = \frac{(1 + \gamma)(1 - \chi)^2(\chi - X_{wd}^*)}{(1 + \gamma\chi)^3(1 - X_{wd}^*)} \quad (\text{S-17})$$

and $L_s = \frac{g\alpha\Delta T K_0 \kappa}{\nu w_{slab}^2}$ is another intrinsic length scale.

5 Model solution

To solve the model equations, one first divides (S-5) by (S-6), and using (S-3), (S-16), and (S-17) one obtains

$$\frac{(1 + \gamma)(1 - \chi)^2(\chi - X_{wd}^*)}{\chi^2(1 + \gamma\chi)^3(1 - X_{wd}^*)} = \frac{D_w}{L_s w_{slab}} \left(\frac{(1 - X_m)X_{wd}^*}{X_m - (1 - X_m)X_{wd}^*} \right)^2 = C_\Gamma \quad (\text{S-18})$$

which yields an equation for χ . Generally, C_Γ is a very small number and thus the only physically viable solution is $\chi \approx 1$ (the other possible solution $\chi \approx X_{wd}^*$ is an artifact of the simplifying assumption that all heat transfer is through percolative convection, and thus there is no heatflow into the slab when porosity $\phi = 0$; this solution is precluded if we add the further complication of accounting for convection outside the solidification zone). An approximate solution is thus $\chi = 1 - (1 + \gamma)\sqrt{C_\Gamma}$, although, in our examination of results, exact solutions are used. That $\chi > X_m$ arises from the fact that water is not easily entrained by slabs and thus accumulates in the melt adjacent to slabs. With the resulting elevated water concentration, diffusion of water into the slab is enhanced and solidification of silicates suppressed (since there is less silicate available to solidify), and thus both entrainment of water and silicate are self-regulated until a steady state is achieved. Of course, if $\chi \approx 1$ then melt near the slab is almost pure water and should be buoyant instead of heavy. However, given the very high viscosity of mantle above this narrow region of the melt zone, it can be easily shown that the buoyant flux of water out of this zone is much smaller than its diffusive flux into the slab.

Once χ is determined, the water fraction of ambient mantle X_a is obtained by using (S-5) along with (S-9) and (S-16). Knowing X_a , the melt fraction f and melt-layer thickness h are determined by (S-1) and (S-9).

Figure 2 of the paper shows results for a standard solution to the model. Parameters used are as follows: $X_{ol}^* = 0.1\text{wt}\%$ (again, the actual water concentration of the solid-phase in an olivine melt is likely to be considerably less than this; however, we use this value as a conservative condition for melting) $X_{wd}^* = 3\text{wt}\%$; $X_m = 10\text{wt}\%$; $g\alpha\Delta T = 0.015\text{m/s}^2$; $\kappa = 10^{-6}\text{m}^2/\text{s}$; $\nu = 3 \times 10^{-4}\text{m}^2/\text{s}$; $\rho_w = 2000\text{kg/m}^3$ (assuming considerable compression of water⁵); $\rho_s = 4000\text{kg/m}^3$; $w_{slab} = 3 \times 10^{-9}\text{m/s}$; $w_0 = 3 \times 10^{-11}\text{m/s}$; $H = 250\text{km}$; and $R = 6000\text{km}$. Results are relatively insensitive to the reference permeability for which we simply use the upper limit of $K_0 = 10^{-4}\text{m}^2$ (ref. 4) given the relatively high connectivity of fluid pathways in partial-solidification regions. Initial water content in the transition zone X_0 is not well constrained and thus we examine solutions over a full range, from X_{ol}^* to $1\text{wt}\%$ (a fraction of the maximum saturation value X_{wd}^* since the water solubility limit at ambient mantle temperatures is likely to be less than the maximum; see main text Methods 3). Water or hydrogen diffusivity in wadsleyite D_w at transition-zone conditions is presently unknown. Olivine hydrogen diffusivity is of order $10^{-8}\text{m}^2/\text{s}$ (ref. 6); however, diffusion of larger cations in wadsleyite is faster than that in olivine by a factor of 10^3 (ref. 7). Therefore it is plausible that hydrogen diffusivity in wadsleyite is as much as 1000 times faster than that in olivine, and thus we consider the possible range $10^{-8}\text{m}^2/\text{s} \leq D_w \leq 10^{-5}\text{m}^2/\text{s}$.

6 Incompatible element balance

The model presented above not only allows for filtering of incompatible elements, but also permits their steady circulation between the melt layer and the transition zone and lower mantle, while being sequestered from the MORB source region. Using our simple circulation model we can estimate the predicted distribution of incompatible-elements in the

mantle. We assume that once the filtering mechanism is established, almost all incompatible elements are retained in the melt layer and sub-410km mantle, while the MORB source region contains a relatively negligible amount. The total mass of a given incompatible element in the mantle must be conserved and thus

$$\rho_s \frac{4}{3} \pi (R_m^3 - R_c^3) C_0 = \rho_s \frac{4}{3} \pi (R^3 - R_c^3) C_a + \rho_s 4\pi R^2 h C_m \quad (\text{S-19})$$

where $R_m \approx 6360\text{km}$ and $R_c \approx 3480\text{km}$ are the mantle and core radii, respectively; C_0 is the present-day bulk mantle average concentration of the given incompatible element (e.g., for ^{238}U , $C_0 \approx 3 \times 10^{-8}\text{kg/kg}$ [ref. 8]); C_a is the average incompatible-element concentration in the sub-410km mantle; C_m is the average concentration in the melt layer; and, for the sake of simplicity, the average melt and solid densities are set approximately equal. We assume that ambient mantle upwelling out of the transition zone has the incompatible element concentration C_a , and since essentially all the incompatible elements go into the melt at 410km, the average melt-layer concentration is approximately $C_m = C_a/f$. The steady-state balance of incompatible element fluxes in the melt layer, i.e., between their injection by the ambient upwelling mantle and their removal by slab entrainment (which returns them to the deeper mantle), yields

$$C_a \rho_s 4\pi R^2 w_0 = \Pi C_m^0 \rho_s 4\pi R \delta_s w_{slab} \quad (\text{S-20})$$

where C_m^0 is the melt's incompatible element concentration at the boundary with the slab, and Π is the incompatible element's partition coefficient between melt and wadsleyite such that ΠC_m^0 is the concentration in the solidification zone (assuming that the solidifying zone entrained by the slab is in local chemical equilibrium with the melt since solidifying crystals are effectively always bathed by circulating melt of concentration C_m^0). As shown below, the near-slab melt concentration C_m^0 is elevated above C_m because incompatible elements do not readily go into the entrained solidifying silicates; they thereby accumulate in the melt until their concentration there and thus in the solidification zone is high enough for slab entrainment to balance their influx from the ambient upwelling. Equation (S-20) can

be simplified further using (S-2), yielding

$$C_a = f(1 - X_m)\Pi C_m^0 \quad (\text{S-21})$$

Equations (S-19) and (S-21), along with the relation $C_m = C_a/f$, lead to

$$\frac{C_a}{C_0} = \frac{f}{\lambda f + \eta} \quad , \quad \frac{C_m}{C_0} = \frac{1}{\lambda f + \eta} \quad , \quad \frac{C_m^0}{C_0} = \frac{1}{\Pi(1 - X_m)(\lambda f + \eta)} \quad (\text{S-22})$$

where $\eta = 3R^2h/(R_m^3 - R_c^3)$ and $\lambda = (R^3 - R_c^3)/(R_m^3 - R_c^3)$. Using sample values of $h = 10\text{km}$, $f = 2\text{wt}\%$ (see Figure 2 of the paper) as well as a conservative partition coefficient $\Pi = 10^{-3}$ (ref. 9), we find representative values of $C_a \approx 0.96C_0$, $C_m \approx 48C_0$, $C_m^0 \approx 54000C_0$, and the incompatible element concentration in the solidification slab entrainment zone is $\Pi C_m^0 \approx 54C_0$. Thus the final average sub-410km mantle concentration C_a is typically a very large fraction of C_0 such that most of the incompatible elements are still kept in the mantle beneath 410km. The average melt layer concentration C_m is not radically elevated above C_0 , and while the concentration in the melt by the slab C_m^0 is elevated thousands of times above C_0 it is still only several hundred to a thousand ppm by mass for ^{238}U concentrations. The concentration entrained by the slab ΠC_m^0 is approximately one ppm by mass for ^{238}U , certainly well beneath saturation values for transition zone materials (given that some upper mantle minerals have uranium and thorium concentrations of 50-150ppm [ref. 9], which are necessarily less than the saturation values for olivine, and well below the saturation values for transition zone materials, given their greater propensity for dissolving incompatible elements).

References

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