

# **The contribution of locally tangential CMB-mantle flow and cold-source subducting plates to ULVZ's formation and morphology**

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## **Key Points:**

- The stable presence of high-density ( $\sim +10\%$ ) partial melts as a cause of ULVZs requires the involvement of the cold subducting plates.
- The morphology of stable ULVZs with flat top and sharp edges are related to the direction and magnitude of the local CMB-mantle flow.
- The flow driven by CMB topography interacting with outer core may be involved in forming mega-ULVZs and ULVZs in seismic-wave cold zone.

## **Abstract**

Ultra-low velocity zones (ULVZs) above the Core-Mantle Boundary (CMB) are significant structures probably connecting the lowermost mantle and the outer core. As "thin patches" of dramatically low seismic-wave velocity, they are occasionally found near the base of mantle plumes and in-or-near high seismic-wave speed regions above CMB. The causes of their morphology-distribution and geodynamics remain unclear, and simulation results of high-density melt diverge from seismic-observations speculation ( $\sim +10\%$ ). We introduce a 2D time-dependent Stokes' two-phase-flow (with

melt-migration) numerical model to investigate the formation and morphological characteristics of ULVZs caused by CMB-mantle tangential flows and a neighboring cold source (subducted plate). We discover that (a) the participation of cold sources with temperature differences between  $\sim 4000$  °K at the plume central regions to  $< \sim 3900$  °K at the plume-cooling mantle region, separated by horizontal distances of about 100 ( $\pm < 50$ ) km are necessary for the stable existence of dense melts with mass-density difference  $> +1\text{-}2\%$  (even  $+10\%$ ) with respect to the surrounding mantle; and additionally (b) an enhanced tangential flow coincident with the internal reverse circulation within the broad plume base (with speeds  $> 3$  times the lowermost-mantle characteristic flow speed); are necessary for higher aspect-ratio-morphology lenses compatible with seismic observations. Our findings suggest that the CMB-mantle tangential flow and/or outer-core interacting with CMB-topography, may be implicated in generating mega-ULVZs, especially if they appear along the edges of LLVSPs and especially when in/near high seismic-speed “cold” zones. We infer a strong link between ULVZs morphology and the dynamical environment of the lowermost mantle and uppermost outer core.

**Keywords:** Ultra-low velocity zone, Core-Mantle Boundary, Mantle plumes, Cold subducting plates, Numerical modeling, Partial melting, Mantle flow

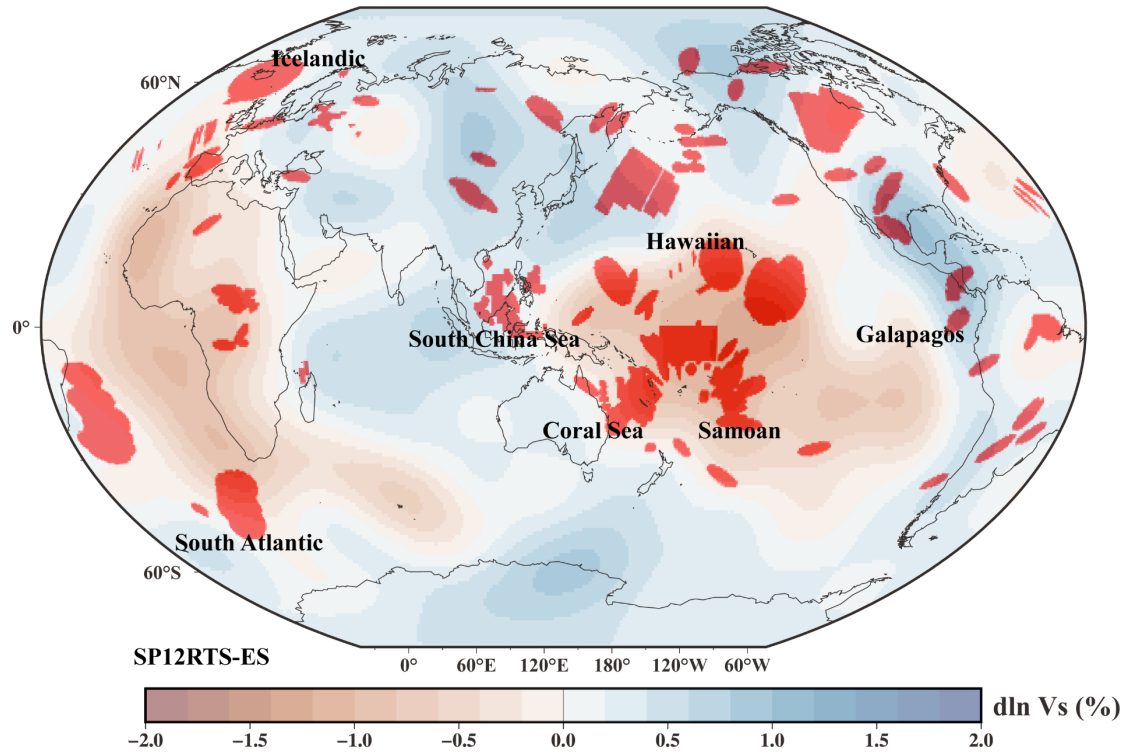
## Plain Language Summary

The Ultra-low velocity zones (ULVZs) above the Core-Mantle Boundary (CMB) are the thin patches structures of rapidly decreasing seismic-wave velocity located at the mantle plume's base and in the seismic-wave high-speed “cold” zone. However, the causes of its formation and morphology remain debatable. We introduce a numerical model to investigate the criteria for the stable existence and formation of high-density melt consistent with observations. By modifying the model bottom boundary conditions, we introduce the effects of CMB-mantle flow and subducting plates as the cold source. According to our findings, the stable existence of high-density melting necessitates the involvement of cold source with lateral temperature difference between  $\sim 4000$  °K at the plume central regions to  $< \sim 3900$  °K at the plume-cooling intermediate mantle region. The ULVZs with a flat top and sharp edges compatible with seismic observations necessitate higher CMB-mantle tangential flow than in the lowermost mantle. Our findings suggest that the flow associated with the CMB topography gradient may be involved in forming ULVZs, especially when they are spread at the superplume margins and in the seismic-wave “cold” zone. Our findings suggest that the ULVZs' morphology is more closely related to the lowermost mantle and uppermost outer core.

## 1. Introduction

The Core-Mantle Boundary (CMB) is the interface between the metallic-liquid outer core and the solid oxide mantle, an important region for heat and mass exchange on Earth. The structural and dynamical characteristics of the CMB are affected by the strong physical differences such as density and viscosity (mantle:  $\sim 5500 \text{ kg}\cdot\text{m}^{-3}$ , core:  $\sim 9900 \text{ kg}\cdot\text{m}^{-3}$ ) and especially viscosity (mantle:  $>10^{12} \text{ Pa}\cdot\text{s}$ , outer-core:  $<10^{-1} \text{ Pa}\cdot\text{s}$ ) (J. W. Hernlund & McNamara, 2015). In the Ultra-low velocity zones (ULVZs), which are 5-40 km-thick zones above the CMB, the seismic wave velocity is locally significantly decreased ( $\sim 10\%$  for P-wave and  $\sim 30\%$  for S-wave) (Garnero et al., 1998). The ULVZs are an important structure connecting the lowermost mantle to the core, similar to the key intermediary crust between the mantle and the surface (J. W. Hernlund & McNamara, 2015). From the seismic waves that pass through the core (e.g., SPdKS, PKKP, and PKP), as well as reflection (ScS, ScP, PcP), diffraction (Pdiff, Sdiff), and scattering at the CMB (Dehant et al., 2022; Yu & Garnero, 2018), it is generally believed that ULVZs with "thin patches" are not globally distributed. Smaller ULVZs have a lateral extent of less than 100 km, larger mega-ULVZs can reach up to 1000 km, and most have a large aspect ratio (Table 1). Many ULVZs are located in the center and/or at the margins of Large Low-Shear-Wave-Velocity Provinces (LLSVPs), but some (a good fraction) are still found in/close-to high seismic-speed "cold zone" (M. Li et al., 2017; Yu & Garnero, 2018) (Figure 1). Less than 20% of the CMB has been explored for ULVZs due to the observational resolution limitations (Z. Li et al., 2022; Rost et al., 2010). The location of some ULVZs imaging is thought to be associated with convergent regions at the mantle plume base (Dannberg et al., 2021), where the ULVZs may be associated with the topography of the CMB at certain wavelengths through gravitational balance (Heyn et al., 2020; Stein et al., 2020). The size and morphology of the ULVZs determined from seismic observations, together with well-constrained high-density contrast, can provide insights into the dynamics and properties of the lower mantle (Rost et al., 2005), the genesis of LLSVPs (Garnero et al., 2016), the nature of global mantle convection (McNamara, 2019), and even give constraints

on outer-core dynamics and its geodynamo (Buffett, 2016; Deschamps & Li, 2019).



**Figure 1. Global distribution of ULVZs.** Red areas represent the detected ULVZs location at/above CMB, data from the seismic observations summarized by (Yu & Garnero, 2017). The background color represents the shear wave velocity anomalies at 2800 km depth from the tomography model SP12RTS (Koelemeijer et al., 2016). Most area-fraction of ULVZs is located in and around low (to null) seismic-speed anomaly regions, but a good fraction (30-40%) of ULVZs are found in/close-to blueish, high seismic-speed "cold" regions.

**Table 1.** Parameters of some ULVZs with good morphological constraints.

Case	Height (km)	Average lateral range/2 (km)	Aspect ratio (lateral range/2/height)	Reference
Hawaiian	30	500	16.7	(Jenkins et al., 2021)
Galapagos	20	300	15.0	(Cottaar et al., 2022)
Icelandic	15	400	26.7	(Yuan & Romanowicz, 2017)
Samoan	15	260	17.3	(Thorne et al., 2013)

<b>Coral Sea</b>	20	350	17.5	(Jensen et al., 2013)
<b>South China sea</b>	10	180	18.0	(Jensen et al., 2013)
<b>South Atlantic</b>	10	90	9.0	(Vanacore et al., 2016)

However, the cause of ULVZs remains controversial. It is generally believed that the ULVZs arise from partial melting and/or chemical-component anomalies, the latter possibly from early BMO (basal magma ocean) crystallization residuals (Labrosse et al., 2007; Pachhai et al., 2022), core-mantle material reactions (Brandon & Walker, 2005; Kanda & Stevenson, 2006; Otsuka & Karato, 2012), material brought by subduction (Dobson & Brodholt, 2005). In most numerical simulations of the lowermost mantle, thermochemical piles have the same rheology as the background mantle (McNamara, 2019), and the ULVZs as a layer of dense chemical components (Beuchert & Schmeling, 2013; Pachhai et al., 2022). Based on seismic observations of the high aspect-ratio low-velocity zone characteristics (Table 1) and the constraints on melt morphology and CMB topography obtained from numerical simulations (Deschamps & Li, 2019; John W. Hernlund & Tackley, 2007), researchers have found that the melt mass-density that fits the observational constraints needs to be larger than that of the surrounding mantle phase. However, excessively high melt density can lead to melt accumulation at the CMB. According to the process of equilibrium of the melt layer under the stirring effect of mantle flow, a maximum difference of  $+50 \text{ kg}\cdot\text{m}^{-3}$  (about +1%) in melt-solid density difference is tolerated (John W. Hernlund & Jellinek, 2010). According to the two-phase flow model (Dannberg & Heister, 2016) and FeO-MgO-SiO<sub>2</sub> pseudo-binary material system (Boukaré et al., 2015), Dannberg et al. (2021) thoroughly examined the role of melting in the origin of ULVZs. They discovered that tolerated melt density difference can be up to  $+120 \text{ kg}\cdot\text{m}^{-3}$  ( $\sim+2\%$ ) (Dannberg et al., 2021), but non-localized and high aspect-ratio melting layers were observed. Considering the seismic observations close to +10% density difference (McNamara et al., 2010; Rost et al., 2005), one question of interest is whether it is possible to enlarge

the melt-solid density difference to a higher range ( $\rho_{melt}-\rho_{solid} \gtrsim +(50 - 120) \text{ kg}\cdot\text{m}^{-3}$ , i.e.,  $(\rho_{melt}-\rho_{solid})/\rho_{solid} > +1\sim 2\%$ ) while the ULVZs melt layer remains stable. What is the mechanism of melt layer formation with a high aspect ratio observed by current seismic observations? Why do some ULVZs appear in/around high seismic-speed “cold” zone, and do the morphology and distribution of ULVZs indicate the involvement of additional dynamical mechanisms regarding lowermost mantle flow?

Most previous studies have modeled the CMB as a temperature-isothermal, velocity-free-slip boundary. Conversely, the CMB region may result from a combination of a hot-and-light mantle plume, dense thermochemical piles, and cold-and-dense subducting/subducted plates (Hansen & Yuen, 1988; Lay et al., 2008). Based on the waveform fitting results of the ScS phase, the formation of the ULVZs may also be related to the thermal effects brought about by the subduction of slabs and the nearby high-velocity zone (Fan & Sun, 2021; Zhao et al., 2017). On the one hand, the presence of a subducting plate pushes low-viscosity material to move, deform and perhaps steepen the boundary of the LLVSPs and/or ULVZs (McNamara & Zhong, 2005; Sun et al., 2019), suggesting that the subducting plates have an effect on the genesis and morphology of the ULVZs. On the other hand, the role of the core side on the ULVZs can also be considered, like the process of outer-core material penetrating into the mantle under dynamic pressure and collapsing with gravitational diffusion (Lim et al., 2021). At the top of the outer core, some studies from seismic observations (Helffrich & Kaneshima, 2010), geomagnetic observations (Buffett, 2014), and geodynamo models (Olson et al., 2017; O’Rourke & Stevenson, 2016) suggest the presence of  $\sim 100$  - 400 km-thick temperature and/or component-stabilized stratified layer (Fearn & Loper, 1981; Mound et al., 2019; van Tent et al., 2020), which affects thermal, chemical, and momentum exchange through the CMB (J. W. Hernlund & McNamara, 2015). Therefore, we suggest altering the velocity and temperature bottom boundary conditions of the model to introduce and incorporate the impact of cold subducting plates and the CMB-mantle tangential flow. This allows us to study the spatial relationships of the corresponding high-density-melt ULVZs in relation to hot and cold

sources, and to provide some constraints on the plausible dynamical conditions at the CMB and the uppermost outer core.

## 2. Model setup

### 2.1. governing equations

We used the finite element software ASPECT (2.4.0) to solve the compressible 2D Stokes' viscous two-phase flow equation (1-4) as well as the temperature field advection-diffusion equation (5) with heat source terms from shear heating, adiabatic heating, and latent heat change from melting/freezing (Bangerth et al., 2022; Dannberg & Heister, 2016; McKENZIE, 1984).

$$\frac{\partial}{\partial t} [\rho_f \phi] + \nabla \cdot [\rho_f \phi \mathbf{u}_f] = \Gamma \quad (1)$$

$$\frac{\partial}{\partial t} [\rho_s (1 - \phi)] + \nabla \cdot [\rho_s (1 - \phi) \mathbf{u}_s] = -\Gamma \quad (2)$$

$$\phi (\mathbf{u}_f - \mathbf{u}_s) = -\frac{k_\phi}{\eta_f} (\nabla p_f - \rho_f \mathbf{g}) \quad (3)$$

$$-\nabla \cdot [2\eta \dot{\epsilon} + \xi (\nabla \cdot \mathbf{u}_s) \mathbf{1}] + \nabla p_f = \bar{\rho} \mathbf{g} \quad (4)$$

$$\bar{\rho} C_p \left( \frac{\partial T}{\partial t} + \mathbf{u}_s \cdot \nabla T \right) - \nabla \cdot k \nabla T = 2\eta (\dot{\epsilon}_s : \dot{\epsilon}_s) + \alpha T (\mathbf{u}_s \cdot \nabla p_s) + T \Delta S \Gamma \quad (5)$$

We still use the compositional advection equation (6) for the porosity and depletion to represent the melt migration process.

$$\frac{\partial C_i}{\partial t} + \mathbf{u}_s \cdot \nabla C_i = \Gamma^i \quad (6)$$

where the subscript  $f$  denotes fluid/melt, the subscript  $s$  denotes solid,  $\phi$  is porosity/melt fraction, and  $\bar{X}$  denotes the averaged quantities  $\bar{X} = (1-\phi) X_s + \phi X_f$ .  $\rho$  is the density,  $\mathbf{u}$  is the velocity,  $\Gamma$  denotes the melt rate given by the compositional equation reaction term,  $k_\phi$ ,  $\eta$ ,  $p$ ,  $\mathbf{g}$ ,  $\dot{\epsilon}$ ,  $\xi$  are the permeability coefficient, the shear viscosity, the pressure, the gravitational acceleration, the strain rate, and the bulk viscosity associated with material dilatation /compaction, respectively. In Equation (5),  $C_p$ ,  $T$ ,  $k$ ,  $\alpha$  are the specific isobaric heat capacity, the temperature, the thermal conductivity, and the coefficient of thermal expansion, respectively.  $S$  is the entropy due to the release or consumption of latent heat.



## 2.2. material model

We simplified the material parameters of the following models to describe the differences in the melt-solid physical properties in terms of the porosity and depletion of the compositional field, in addition to utilizing the "Dannberg" model parameters as the reference model for comparison (Dannberg et al., 2021). The detailed material parameters are as follows.

**Table 2.** Material properties of the numerical models.

	parameter	value	unit
	Melting time scale	$10^3$	yr
<i>depletion</i> <sup>a</sup>	Depletion density change	-180	$\text{kg}\cdot\text{m}^{-3}$
	Depletion solidus change	216	$^{\circ}\text{K}$
	Maximum Depletion viscosity change	$10^4$	—
<i>viscosity</i>	Reference bulk viscosity $\xi_{\text{ref}}$	$10^{23}$	$\text{Pa}\cdot\text{s}$
	Reference melt viscosity $\eta_{\text{f, ref}}$	10	$\text{Pa}\cdot\text{s}$
	Reference shear viscosity $\eta_{\text{ref}}$	$10^{23}$	$\text{Pa}\cdot\text{s}$
	Exponential melt weakening factor	23	—
<i>initial melt state</i>	Pressure solidus change $\Delta T_{\text{p}}$	$-10^{-8}$	$\text{Pa}^{-1}$
	Surface solidus $T_{\text{sol},0}$	5100	K
	Difference between liquidus and solidus $T_{\text{liquid}}-T_{\text{solid}}$	1900	K
<i>permeability</i>	Reference permeability $k_{\Phi, \text{ref}}$	$5\times 10^{-12}$	$\text{m}^2$
	Gravity acceleration $\mathbf{g}$	10.68	$\text{m}\cdot\text{s}^{-2}$
<i>density</i>	Reference melt density $\rho_{\text{f, ref}}$	5800	$\text{kg}\cdot\text{m}^{-3}$

Reference solid density $\rho_{s, \text{ref}}$	5500	$\text{kg}\cdot\text{m}^{-3}$
Melt compressibility	$1.6\times 10^{-12}$	$\text{Pa}^{-1}$
Solid compressibility	$1.6\times 10^{-12}$	$\text{Pa}^{-1}$
<i>thermal dependence</i>		
Reference temperature $T_{\text{ref}}$	298	K
Reference specific heat $C_{p, \text{ref}}$	1230	$\text{J}\cdot\text{kg}^{-1}\cdot\text{K}^{-1}$
Thermal conductivity $k$	8.5	$\text{W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$
Thermal expansion coefficient $\alpha$	$1\times 10^{-5}$	$\text{K}^{-1}$
Thermal viscosity exponent	10	—
Thermal bulk viscosity exponent	10	—

<sup>a</sup> Based on an approximate estimate from the Dannberg model setup.

When a phase change occurs,

$$\phi_{\text{equilibrium}} = \frac{T - T_{\text{sol}}}{T_{\text{liq}} - T_{\text{sol}}} \quad (7)$$

$$T_{\text{sol}} = T_{\text{sol},0} + \Delta T_p p + \Delta T_c C_{\text{depletion}} \quad (8)$$

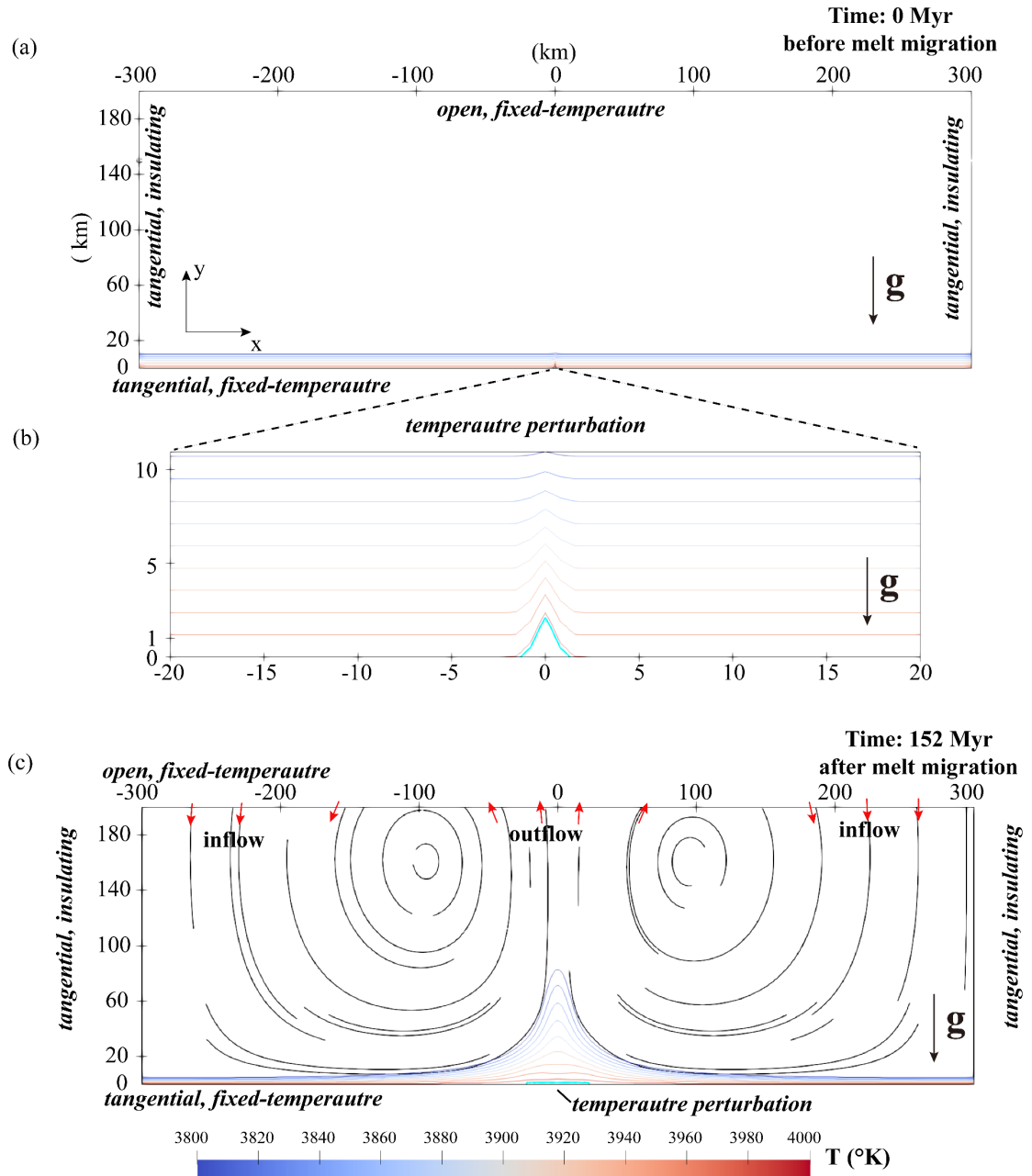
where  $C_{\text{depletion}}$  is composition depletion,  $\Delta T_c = 200$  °K.

Here, the first parameter melting time scale is set to be smaller than advection time step to accurately resolve the melting/freezing process. The difference in Fe-Mg distribution in the solid-melt described by depletion (indicating the residue after melt migration) leads to variations in density and melt fraction. We refer to the physical parameters of the "Dannberg" model and let the distribution coefficient  $K_D = \frac{X_{\text{Fe}}^S X_{\text{Mg}}^L}{X_{\text{Fe}}^L X_{\text{Mg}}^S}$  remains constant (0.23) during the model simulation. We do not explore the viscosity change in this model, so we keep the "exponential melt weakening factor" fixed, making its shear viscosity near the lowermost mantle  $10^{19}$ - $10^{22}$  Pa·s (Ricard, 2015). The three parameters of the initial melt state together describe the initial and subsequent melting area. Combined with the geothermal line, we make the model in the initial stage ~15 km thick, and the maximum value is 0.16. The Clapeyron slope employed here is negative (Beuchert & Schmeling, 2013), and we investigated the impact of positive and

negative slopes separately in Section 4.2. We used the same compression coefficient for both solid and melt to conveniently regulate the variation of melt-solid density, and only altered the reference density during the subsequent study. The specific heat in the thermal parameters changes in the model with temperature and melt fraction. Temperature, pressure, and melt fraction all affect the latent heat in the heat source term.

We use a 2D Cartesian box model of 600 km (horizontal)  $\times$  200 km (vertical) to model the lowermost mantle, see Figure 2. The initial temperature profile is an adiabatic profile, and a temperature perturbation (before melt migration is +50 °K, after that is +10 °K) is continuously applied at the bottom center of the model (0 km) to trigger a mantle plume. The porosity and depletion represented by the compositional field are both 0 in the initial stage.

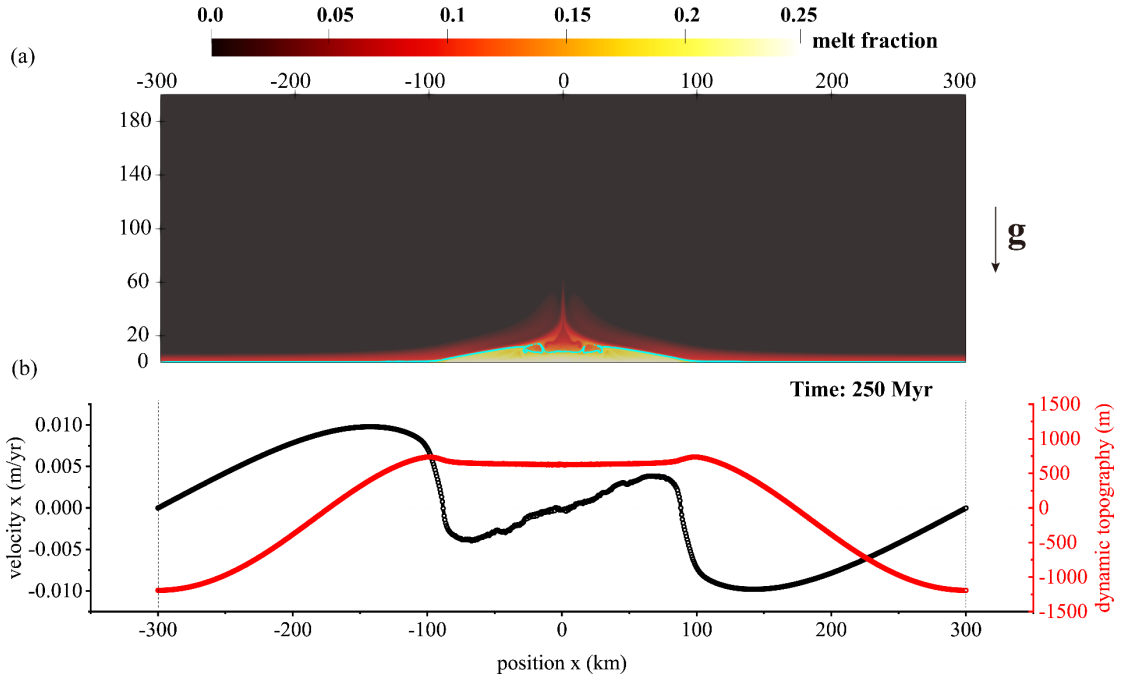
As seen in Figure 2, our computational model is symmetric about the central vertical line  $x = 0$ . In real-Earth, different regions near the mantle plume will not have the exact same thermal-chemical structure (such as subducted plates) as here prescribed. The reason we continue to use the a full-symmetrical model, rather than using just half of it (any of the sides  $x \leq 0$  or  $x \geq 0$ ), is to verify and illustrate the accuracy of the results from the numerical modeling, that is, that any apparent asymmetry is beyond the scope of our discussion. More so, in later parts of this article, we extract the symmetric part of the computation output, by taking averages (arithmetic mean) about  $x=0$  for some selected variables; that symmetric part should have smaller numerical errors.



**Figure 2. Reference model setup. (a) Initial condition setup before melt migration (150 Myr).** The surrounding symbols represent boundary conditions, where the reference model has a fixed (in time) temperature (here 4000  $^{\circ}\text{K}$ ) and tangential flow at the bottom boundary. The colored contour denotes the partial temperature distribution (3800–4000  $^{\circ}\text{K}$ ), where a sustained temperature perturbation (before melt migration, the maximum is +50  $^{\circ}\text{K}$ , after that is +10  $^{\circ}\text{K}$ ) is applied in the bottom center to trigger the mantle plume. **(b) The initial temperature perturbation closeup.** The perturbation maximum decays exponentially as the square of the distance from the bottom boundary center. **(c) Setup after melt migration (150 Myr).** The black streamlines represent the (solid) velocity direction, and sparseness has no special meaning. Red arrows represent the flow direction at the top open boundary. The blue line represents the contour of the fixed melt fraction (0.16).

### 2.3. Boundary condition

The left and right boundaries of the model are adiabatic and tangential flow boundaries, i.e., free-slip (zero shear stress) and no-flow-through (zero normal velocity). The upper boundary is a fixed-temperature and open boundary. The bottom boundary represents the fixed (in time) CMB with a pressure of 136 GPa and a temperature of 4000 °K (Dziewonski & Anderson, 1981), except for a sustained temperature perturbation at the center triggering mantle plume. The bottom velocity boundary of the reference model is also a tangential flow boundary (Figure 2). Throughout this article, when we write about the velocity in the model, or the velocity in the real Earth's mantle, we refer to the velocity of the solid phase of the mantle. Exceptions regarding melt are explicitly stated. We nevertheless state 'solid velocity' in a few crucial cases.



**Figure 3.** (a) The melt fraction of the reference model ( $\rho_{\text{melt}} - \rho_{\text{solid}} = +300 \text{ kg}\cdot\text{m}^3$ ) at 250 Myr after the initial condition (which is the time when the subsequent experimental model boundary parameters start to change). The blue line is the same as Figure 2. (b) The model tangential velocity (black, along  $x$ -direction) and dynamic topography (red) distribution on the bottom boundary (CMB) at 250 Myr, it is important to note that we use the normal stress  $\sigma_{\text{tr}}$  as the equivalent for dynamic topography  $h = \sigma_{\text{tr}} / [(\mathbf{g} \cdot \mathbf{n}) \cdot (\rho - \rho_{\text{core}})]$  (Bangerth et al., 2022; McKenzie et al., 1974). The model is, within numerical errors, symmetric with aspect to its centerline, with velocities and topography mirrored with respect to  $x=0$ .

The subsequent model boundary setting is based on the following.

### **2.3.1 Bottom boundary temperature**

As mentioned in the introduction, considering the heat-mass exchange at the CMB, we introduce the influence exerted by a cold source, such as subducting/subducted plates in the mantle, by setting a non-uniform mantle-bottom temperature boundary in the following model. Given that some ULVZs are located in seismic cold zones and at the edge of the Pacific or Afro-Atlantic LLVSPs (Garnero & McNamara, 2008), this could suggest the presence of long-lasting cold sources. Then, according to previous estimates of the lateral temperature variation in the lowermost mantle, the peak temperature difference between the mantle plume base and surrounding lower mantle is not expected to be more than 500 °K (Davies et al., 2015; Deschamps & Li, 2019; Solomatov & Moresi, 2002; WATSON & McKENZIE, 1991). Although the lateral temperature variation at the top of the outer core does not exceed ~1 °K (Mound et al., 2019), considering the stronger heat exchange within the outer core (owing to high thermal conductivity) than in the mantle, and in reference to the  $\pm 100$  °K setting in previous work (Aubert et al., 2007), we set the peak lateral temperature difference between cold source location and normal ambient mantle at the bottom boundary to be 0, -100, -200, -300 °K. This would result in both a cooling effect on the local ambient mantle outside of the mantle plume and the cooling of the plume itself within a few tens of kilometers (<50 km) of the plume edge (Figure S1).

### **2.3.2 Bottom boundary velocity**

As for velocity boundary, the same as previous studies, we set the velocity-free-slip bottom boundary in reference model (Figure 3). Under the zero-shear stress assumption, this leads to CMB velocity that is generated entirely by mantle convection as well as gravitational action. However, previous studies results show that this is not sufficient to explain the high-density ULVZ morphology distribution, so in the following section we will introduce other factors that contribute to the CMB velocity. Previous observations reveal that dense material piles within the plume spontaneously form internal reverse circulation, allowing mantle flows along the CMB to converge at the

edge of the plume (Kellogg & King, 1993; Luo et al., 2001; McNamara, 2019). The drag force driven by CMB topography, as well as the net horizontal electromagnetic force from on the outer core (Dehant et al., 2022; Glane & Buffett, 2018), may affect the internal reverse circulation.

In the first part of this study (section 3.1), our reference model, utilizing CMB dynamical BCs of zero flow through and zero shear stress, found a self-consistent convecting-mantle flow, that of course contained and produced a dynamically-consistent mantle velocity field at the CMB. In the second part (after section 3.1), we prescribe/impose Dirichlet BCs on the mantle velocity field at the CMB.

For this Dirichlet velocity field, we firstly need to note the following: The mantle mass-elements' velocity distribution and speeds at the CMB, the proper Dirichlet boundary velocity field, although seemingly somewhat arbitrary or artificial, is based on the dynamically-consistent mantle flow computed in the reference model. Therefore, this CMB-mantle Dirichlet velocity field adequately imitates the resulting velocity field of a system in which the velocity is a consequence of self-consistent pressure and viscous forces operating during convection: The convecting-mantle pressure field and viscous-field horizontal forces move the mantle-CMB mass-particles at those velocities. Thus in principle, our second-part model contains Dirichlet boundary velocities that are approximately consistent with a reasonable model setting.

Additionally, if externally-driven velocities are considered, the liquid-iron outer-core may exert forces on the lower-most mantle thus affecting its velocity field. We will quickly review that (a) CMB topography and (b) possible magnetic forces, can potentially have non-negligible effects influencing the velocity field at the mantle CMB.

Here, we vary the bottom tangential traction to experiment with how large a force source is required to produce localized CMB-mantle flow velocities of the magnitude comparable to the lower mantle characteristic convective speed ( $\sim 1$  cm/yr (Flament et al., 2017)). The bottom boundary traction model simulations show that to reach velocities of that magnitude, based on the outer-core-flow drag force formula in plane laminar flow  $F_{drag} = c_D \frac{\rho}{2} u^2 b l$  (Schlichting & Gersten, 2017), where at a modest

Reynolds number (here of about  $Re \sim 10^7 - 10^8$ ), considering outer-core parameters  $\eta = 0.01$  Pa·s,  $u = 5 \times 10^{-4}$  m/s (Jones, 2015),  $l$  as the half plume width, the drag force must be increased by a factor of  $10^5$  (Figure S2). We assume that the core-mantle mass exchange layer (a region where chemical exsolution is upward from the outer core and downward from the mantle, and accumulated material may reside for different amounts of time), at the uppermost outer core beneath the CMB, may have a higher viscosity and resulting local drag effect facilitated by CMB topography. Given the length  $l$  of  $x \times 10^1 \sim 10^2$  km, and take the drag coefficient  $c_D = 24/Re$  at a small Reynolds number ( $< 10^3$ ) where  $F_{drag} = 12\eta ul$ , a sufficient non-essential condition is that the thin mass exchange layer viscosity could reach  $10^3 \sim 10^5$  Pa·s (an intermediate value between outer-core and lowermost mantle).

After these considerations, during the subsequent parts of this study we setup a Dirichlet-type velocity boundary condition at the mantle-CMB, whose horizontal-component distribution is prescribed to have the form of the velocity distribution obtained in the free-slip-BC simulation (Figure 3) and 0 in the vertical  $y$ -direction, meaning that this Dirichlet velocity field simulates the resultant velocity field dynamically obtained from the tangential BC, which is consistently related to the internal reverse circulation and furthermore to the CMB dynamic topography. Naturally, applying traction ('Neumann' velocity) at the bottom boundary will produce slightly different results than applying "Dirichlet" velocity (see the bottom horizontal velocity in Figure 3b and Figure S2), but let's start with the model of the applied horizontal velocity that is more closely aligned with the reference free-slip-BC model.

#### 2.4. Other model settings

In order to maintain the calculation stability at the beginning of the modeling, we also divided the simulation process into two stages (Dannberg et al., 2021). In the initial stage of 0-150 Myr, we prevented melt migration from happening by increasing melt scaling factor ( $10^{20}$ , equivalent to reducing the permeability coefficient virtually to 0), and allowed the mantle plume to form under the initial temperature perturbation. We start to apply melt migration in the second stage (that is, a smaller melt scaling factor



of  $10^{-8}$ ) when the average temperature and average velocity have reached a steady state. The minimum size of the model grid is  $781 \text{ m} \times 781 \text{ m}$  after 8 adaptive refinements, and the minimum total time step is  $\sim 7000 \text{ yr} - 13000 \text{ yr}$ , the melting (migration) time step is  $1000 \text{ yr}$ , which satisfies reasonable resolution requirements of ULVZs.

Let's briefly summarize the idealizations and simplifications we adopted for the models in this study, (a) We utilize a bottom boundary conditions to represent our conceptual framework rather than explicitly introduce the cold subducted plates and the underlying dense liquid outer core. (b) For evaluating different boundary conditions, we employ simplified material properties associated to the melt migration model. We then compare the findings of our model to those of an unsimplified-properties (Dannberg) model under the same boundary conditions. (c) We utilize a 2D symmetric (along  $x=0$ ) model thus our discussion of boundary-conditions effects will not cover asymmetric outcomes; and although this limits the discussion it allows a much simpler dynamics for easy understanding.

### **3. Results**

#### **3.1. The impact of melt-solid mass-density difference on melt formation**

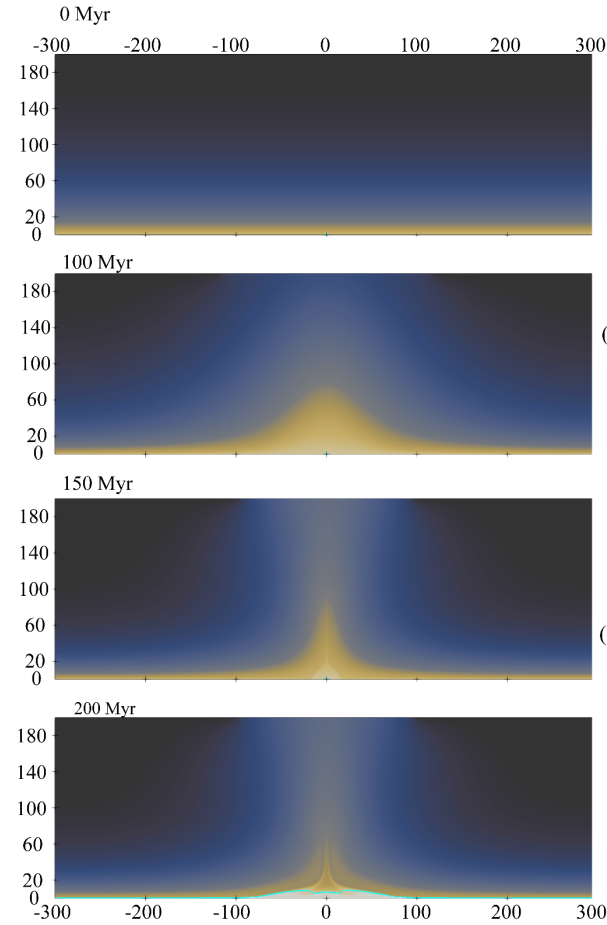
First, we compared the "Dannberg" model with our reference model while simplifying the material model (Figures 2 and 3) in order to control variables. Then, we compare the reference model results with the subsequent experimental model with modified bottom boundary conditions.

We refer to the model with the simplified material parameters, tangential flow, and constant temperature bottom boundary as "ref" in Figure 2. The binary melt system with the same bottom boundary is referred to as "Dannberg" (Dannberg et al., 2021).

The experimental model " $\Delta T_{200} \Delta v_{0.03}$ " depicts the model with a modified bottom boundary, whose lateral extent and its velocity distribution (with direction-and-sense) are identical to those obtained in the reference model (Figure 3), in which the CMB-mantle mass moves away from the center within the mantle plume and towards the center outside; in model " $\Delta T_{200} \Delta v_{0.03}$ " these velocities are Dirichlet-prescribed. The peak temperature difference between cold source location and normal ambient mantle

is  $-200\text{ }^{\circ}\text{K}$  ( $T_{\text{bottom, peak}} - T_{\text{bottom, ambient}}$ ), and the peak horizontal velocity is  $3\text{ cm/yr}$  (that is  $30\text{ km/Myr}$ ) ( $v_{\text{peak}}$ ). Their specific distribution along the bottom boundary is shown in Figures 7d and 7b.

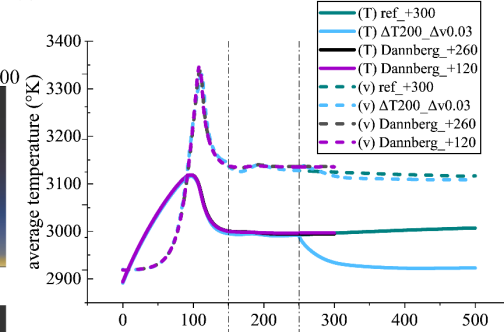
(a)



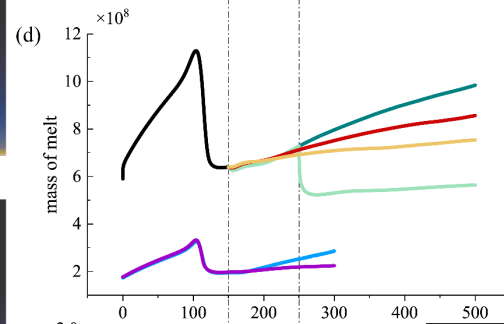
shear viscosity (Pa·s)

$1e+18$   $5e+18$   $1e+19$   $5e+19$   $1e+20$   $5e+20$   $1e+21$   $5e+21$   $1e+22$   $1e+23$

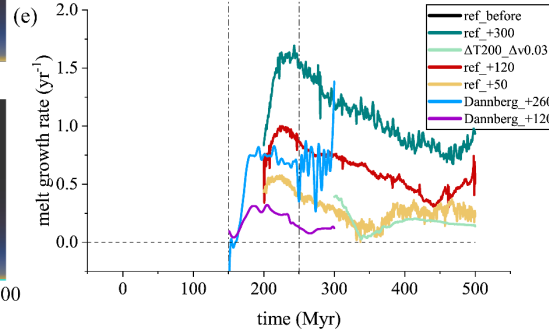
(c)



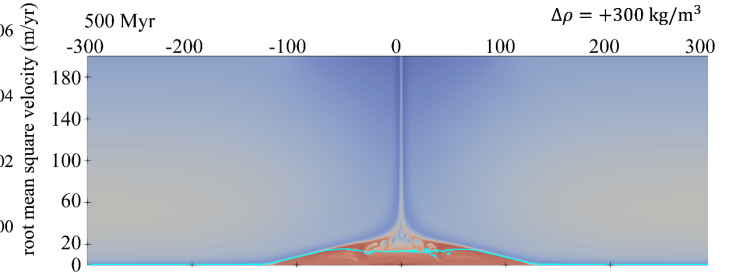
(d)



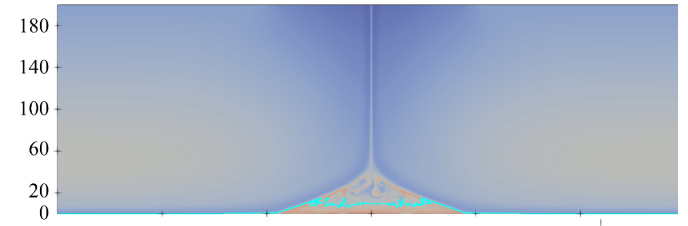
(e)



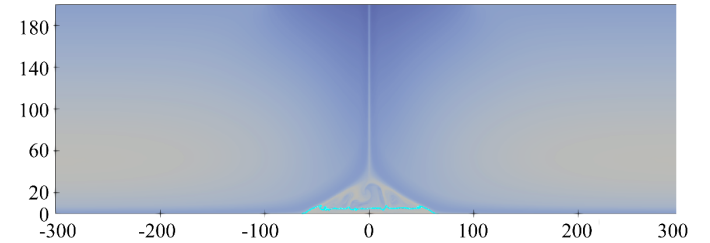
(b)



500 Myr

 $\Delta\rho = +120 \text{ kg/m}^3$ 

500 Myr

 $\Delta\rho = +50 \text{ kg/m}^3$ density (kg/m<sup>3</sup>)

5400 5450 5500 5550 5600 5650 5700

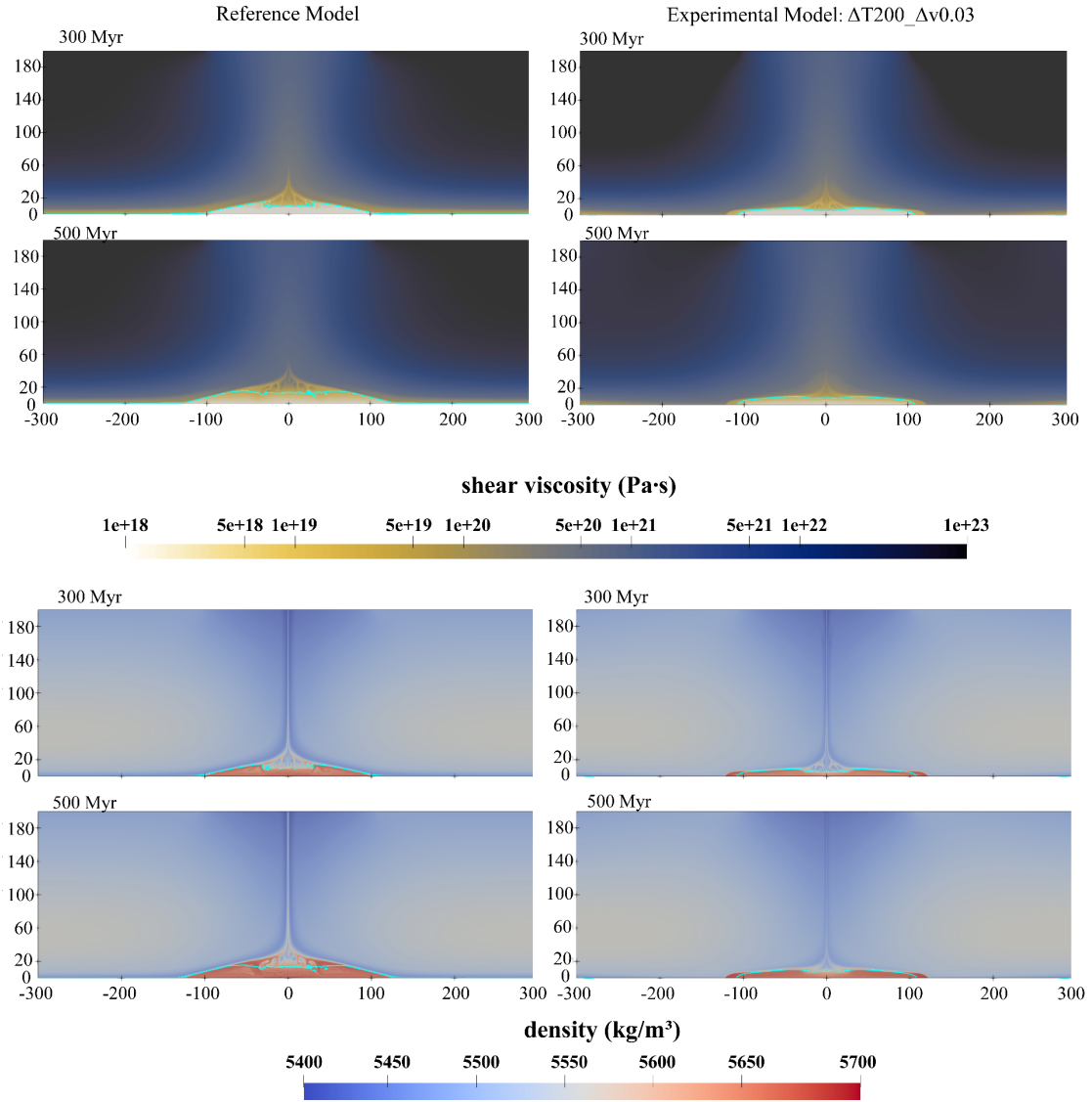
**Figure 4. Comparison of the results of different melt-solid density difference models.** (a) Reference model evolution shown by shear viscosity distribution, blue contour as in Figure 3. **(b) Reference model comparison of the melt-solid density differences  $\Delta\rho$**  ( $\rho_{\text{melt}} - \rho_{\text{solid}} = +50, +120, +300 \text{ kg}\cdot\text{m}^{-3}$ ) at the simulated end time (500 Myr), shown by density distribution ( $\bar{\rho} = (1-\phi)\rho_{\text{solid}} + \phi\rho_{\text{melt}}$ ,  $\phi$  is melt fraction), blue contour as in Figure 3. Center column: **The evolution of (c) the average velocity (right axis), average temperature (left axis) over the entire study area, (d) the total melt mass, and (e) the melt growth rate.** The number after the models' name represents the melt-solid density difference ( $\text{kg}\cdot\text{m}^{-3}$ ). "ref" represents the reference model (Figure 3), "ref\_before" is the stage before melt migration (150 Myr), "Dannberg" is the model from (Dannberg et al., 2021), " $\Delta T_{200\_}\Delta v_{0.03}$ " is the experimental model with the density difference of  $300 \text{ kg}\cdot\text{m}^{-3}$  and the non-uniform constant bottom boundary, with  $\Delta T = T_{\text{bottom, peak}} - T_{\text{bottom, ambient}} = -200 \text{ }^{\circ}\text{K}$  and  $\Delta v = v_{\text{bottom, peak}} = 0.03 \text{ m/yr}$ . The detailed distribution is shown in Figures 7d and b. We choose the melt growth rate of "Dannberg\_+120" as the criteria to evaluate whether the melt has reached stability in Figure 6.

Figure 4a shows the evolution of the shear viscosity field for the "ref+300" model. The low-viscosity melt initially generates at the bottom of the plume and then spreads out to the sides after the melt migration occurs, as shown by the yellow backdrop and blue contour. Figure 4b displays the melt density distribution (density  $\bar{\rho} = (1-\phi) \rho_{\text{solid}} + \phi \rho_{\text{melt}}$ ,  $\phi$  is melt fraction) for different density differences ( $\Delta\rho = \rho_{\text{melt}} - \rho_{\text{solid}}$ ) of the "ref" model at the simulated end time (500 Myr). As the melt-solid density difference rises, the red high-density melt structure becomes increasingly wider to the sides. Similar to the findings of previous studies, the lesser positive density difference will make it easier for it to be entrained in the rising mantle flow, and the negative density melt will allow it possible for it to ascend through the mantle without accumulating at its base (Garnero & McNamara, 2008).

Except for the total amount of melt (Figure 4d), the results of our reference model versus the "Dannberg" model reveal no significant difference (Figure 4c). Figure 4c depicts the evolution of average velocity and temperature over the entire study area. The mantle flow in the model no longer varies considerably following the development of the mantle plume (150 Myr, black dashed line on the left), except that the average temperature decreases after the bottom cold source is applied (250 Myr, right black dashed line). Figure 4d depicts the results of the total melt mass growth over time. Our reference and "Dannberg" models both show that the smaller the density difference, the easier the melt tends to stabilize.

Although the total melt mass obtained from the "ref" model ended up being 4-5 times greater than that obtained from the "Dannberg" model, it does not affect our study of their melt variation tendencies, as the evolution of the melt growth rate (Figure 4d and 4e). In addition, using the stable "Dannberg (+120)" shown in purple as a baseline, we can see that the melt of the "ref (+50)" with lower positive density difference, as well as the experimental model " $\Delta T_{200} \Delta v_{0.03}$ " with a cold source and bottom tangential flow, eventually reaches stability. Then, we take the melt growth rate of "Dannberg (+120)" as the criteria to evaluate whether the melt has reached stability in the subsequent section 4.1.

### 3.2. The impact of bottom boundary setup on melt morphology



**Figure 5.** The comparison of reference and experimental model at 300 and 500 Myr, shown by shear viscosity (top) and mass density (bottom). "ref\_+300" model (left column) and " $\Delta T200_{\Delta v0.03}$ " (right column) are the same as Figure 4, the blue line as in Figure 3. The right-column (prescribed Dirichlet-type velocity bottom boundary condition) model's high-density, low-viscosity melt region has a flatter top and steeper edges than the left-column reference model.

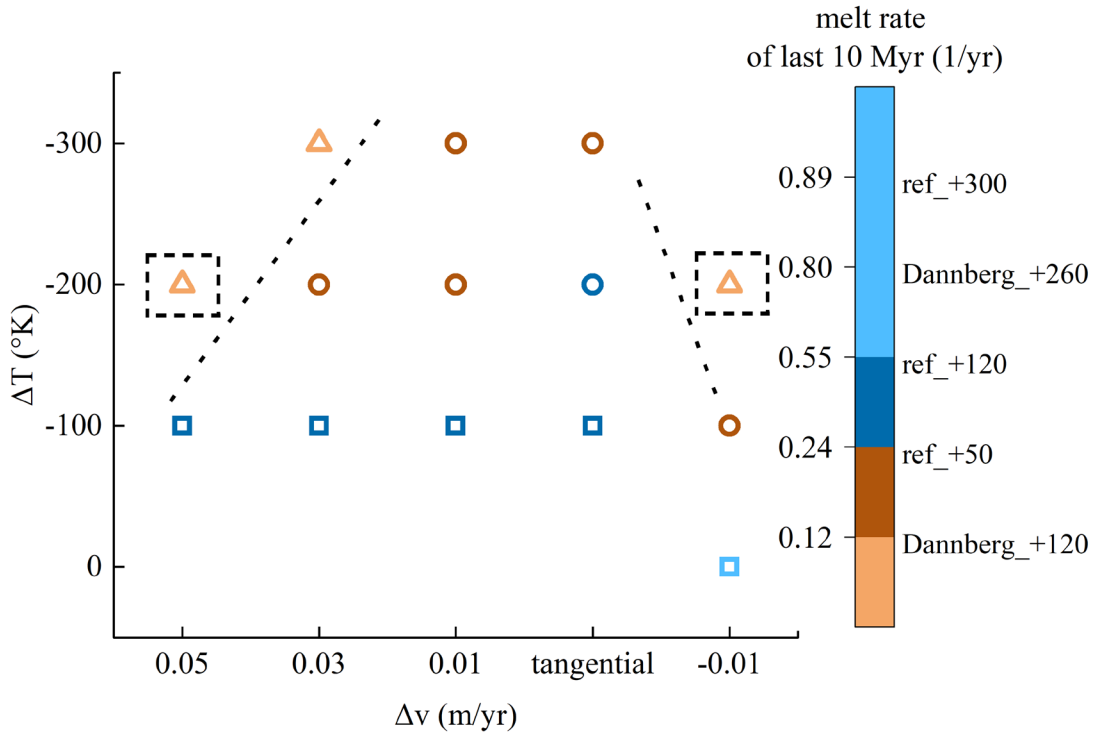
Figure 5 depicts the model's density and shear viscosity distributions without (left) and with (right) changing the bottom boundary conditions at two instants, revealing that after the application of cold source as well as the bottom tangential flow, the model produces a melt with sharp edges and flat tops similar to those observed by seismic

(Rost et al., 2005, 2006), while the aspect ratio of the melt layer increases in the latter. Previous interpretations of the steep edges of the LLVSP and ULVZs have emphasized the pushing effect of the subduction plate with mantle flow (Davies et al., 2015; John William Hernlund & Bonati, 2019). Our findings could indicate that the thermal effect of the subduction plate as a cold source between it and the ULVZs is sufficient to generate a melt layer with sharp edges, in which internal tangential flow, enhanced by the CMB topography and uppermost outer core, also plays a significant role.

## 4. Discussion

### 4.1. Stable conditions for high-density melts

We assume that the conditions of this distribution near the edge of the LLVSPs allow for lengthy durations of existence (perhaps  $> 100$  Myr), as mentioned in Section 2.3. Hence in this section, the boundary values are held constant in the parametric analysis. To explore the influence of varying bottom temperature and velocity parameters on the melt growth rate, we fixed the melt-solid density difference at  $+300 \text{ kg}\cdot\text{m}^{-3}$ , as shown in Figure 6.



**Figure 6. Phase diagram of melt growth-rate for the models' bottom boundary setups.** The model mass-density differences ( $\rho_{\text{melt}} - \rho_{\text{solid}}$ ) are fixed at  $+300 \text{ kg}\cdot\text{m}^{-3}$ .  $\Delta T$  is the peak value of

the applied bottom temperature difference, between the ‘cold-source’ and the ambient ( $\Delta T = T_{\text{bottom, peak}} - T_{\text{bottom, ambient}}$ ), separated by horizontal distance of about 100 km, and defines the rows in the plot.  $\Delta v$  represents the peak value of applied bottom-boundary velocity (Dirichlet-type) ( $\Delta v = v_{\text{bottom, peak}}$ ) and defines the columns in the plot. Note that for comparison, we replaced the " $\Delta v = 0$ " with the "**tangential**" (Neumann-type) velocity boundary as in the reference model (Figure 3). Each element represents one single simulation. Colors indicate the average melt growth rate within 10 Myr before the simulated end time (500 Myr). The symbols in the right-side legend indicate the classification criteria derived from the reference model results (Figure 4e). The category of melt-stability discrimination: Orange triangles indicate that model melt reached a stable state (top left and right corners), blue rectangles indicate unstable states and brown circles are transition states models. The simulations enclosed by dashed-line squares are used in Figure 7.

In Figure 6, the vertical coordinates represent the lateral temperature difference peaks between a mantle neighboring cold source and normal ambient mantle ( $\Delta T = T_{\text{bottom, cold peak}} - T_{\text{bottom, ambient}}$ ) of 0, -100, -200, and -300 °K. The horizontal axis indicates the velocity setup (Dirichlet-type) with labels being positive for flow in the same direction of the tangential flow model (Neumann-type) (Figure 3), with maximum values ( $\Delta v = v_{\text{bottom, peak}}$ ) of 0.01, 0.03, 0.05 m/yr, and a single negative value of -0.01 m/yr (meaning flow in the opposite direction to that of reference). The melt growth rate for the last 10 Myr of the simulation is represented by the colors in Figure 6 and is depicted in Figure 4e. The categorization criteria for determining if the melt reaches stability are presented on the legend text. Based on previous studies (Dannberg et al., 2021; John W. Hernlund & Jellinek, 2010) and the melt results in Figures 4d and 4e, we use the melt rates of the "Dannberg+120" and "ref+50" models as the cut-off. We use orange triangles to represent the model melt finally stabilizing, blue rectangles to represent the model melt failing to stabilize, and brown circles to represent the transition zone.

It indicates that the melt stabilization zone lies in the phase diagram's upper left positive-flow-velocity region and the upper right negative-flow-velocity region. It means the greater the temperature differences and velocity when the velocity direction is the same as the "ref" model (positive), the easier the melt stabilizes. Additionally, a maximum velocity of 0.01 m/yr can stabilize the melt when the velocity is reversed



(negative). The cold source reduces the melt fraction, and the CMB-mantle tangential flow increases the cooling effectiveness. Furthermore, stronger flow facilitates the migration of the melt towards localized "cooling zone". In the absence of a cold source, even a strong bottom tangential flow is unable to stabilize the melt. Our findings show that, in order to stabilize a melt that has a higher density ( $\rho_{\text{melt}} - \rho_{\text{solid}} > 50\text{-}120 \text{ kg}\cdot\text{m}^{-3}$ ), a cold source is necessary, with the corresponding lateral temperature difference between  $\sim 4000 \text{ }^\circ\text{K}$  at the plume central regions to  $< \sim 3900 \text{ }^\circ\text{K}$  at the plume-cooling intermediate mantle region, separated by horizontal distances of  $\sim 100 \text{ km}$  (approximately as shown in Fig 7).

When the density difference between the solid and the melt is up to  $\sim +10\%$  ( $(\rho_{\text{melt}} - \rho_{\text{solid}})/\rho_{\text{solid}}$ ), the stable presence of melt still requires a cold source with a temperature difference absolute value  $> 100 \text{ }^\circ\text{K}$  (Table 3). However, the melt growth rate actually decreases for the same boundary setup when the density difference approaches  $\sim +10\%$ , indicating that the boundary conditions' lower limit can relax for additional increases in density difference. We speculate that this may be because the Rayleigh number ( $Ra = \rho g \alpha \Delta T h^3 / (\eta \kappa)$ ) increases further through the density, which denotes enhanced local convection within the ULVZs and morphology stability of the melt.

**Table 3.** The model melts growth rate <sup>a</sup> comparison regarding the melt-solid density difference ( $\rho_{\text{melt}} - \rho_{\text{solid}} = +300, +500 \text{ kg}\cdot\text{m}^{-3}$ ) under different bottom boundary conditions (Figure 6).

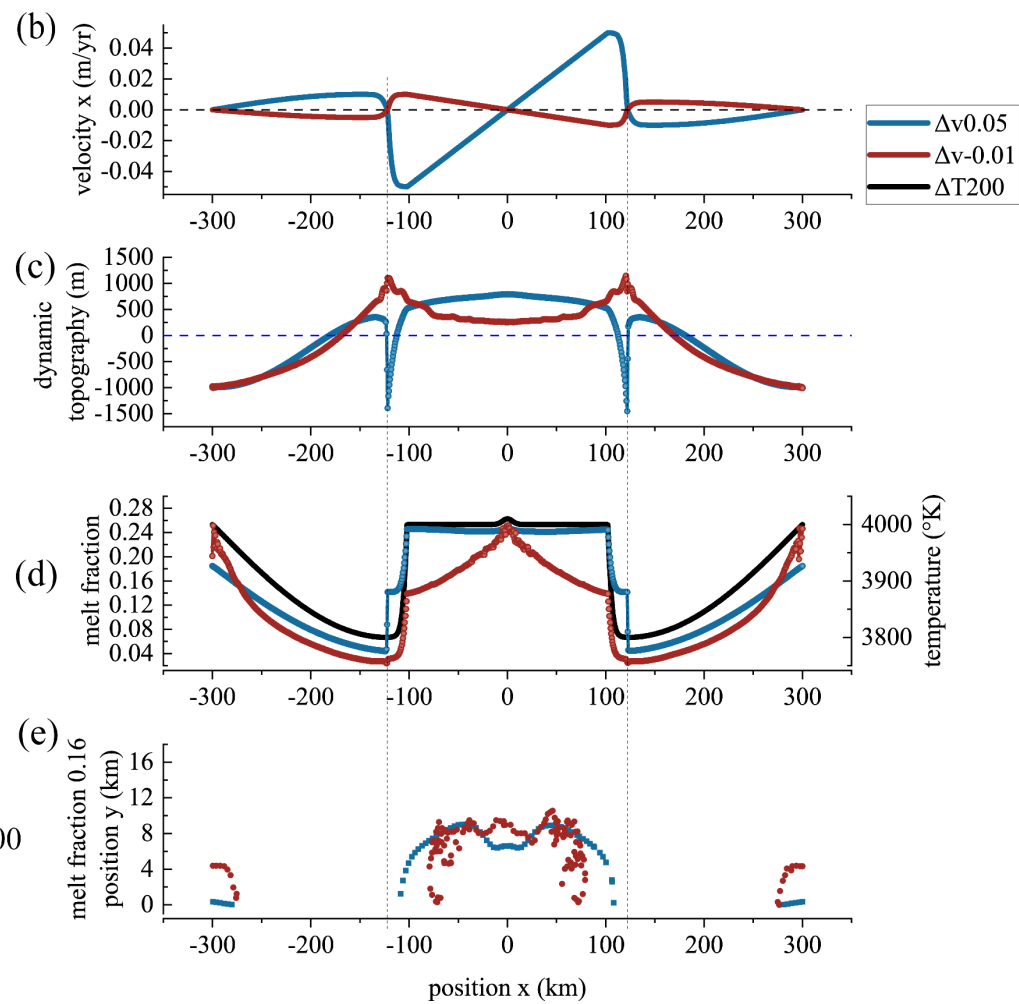
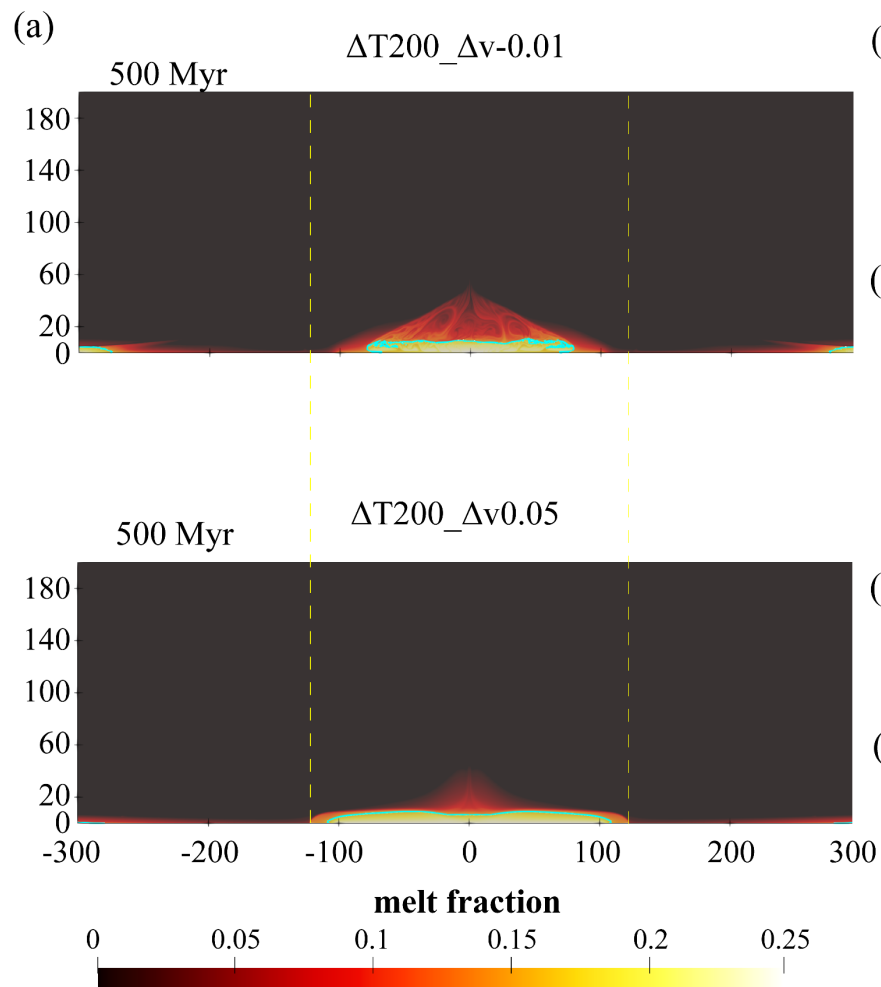
Density difference $+300 \text{ kg}\cdot\text{m}^{-3}$			
Bottom boundary condition	0.05 m/yr	0.03 m/yr	0.01 m/yr
-300 K		<b>0.107</b>	0.125
-200 K	<b>0.109</b>	0.147	0.208
-100 K	0.291	0.331	0.425
Density difference $+500 \text{ kg}\cdot\text{m}^{-3}$			
Bottom boundary condition	0.05 m/yr	0.03 m/yr	0.01 m/yr
-300 K	<b>0.057</b>	<b>0.064</b>	<b>0.080</b>
-200 K	<b>0.109</b>	<b>0.111</b>	0.158

-100 K	0.362	0.426
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<sup>a</sup> The stable (bolded) upper limit of growth rate is the same as Figure 6 ("Dannberg\_+120" model:  $\sim 0.12 \text{ yr}^{-1}$ ).

#### 4.2. Morphological characteristics of the stabilized melt

Since both positive and negative velocities can mechanically stabilize the melt, as described in Section 4.1, we selected the two models " $\Delta T200_{\Delta v 0.05}$ " and " $\Delta T200_{\Delta v -0.01}$ " ringed by dashed circles in Figure 6 to study the differences in the generated melt morphology.



**Figure 7. Example model results illustrating the effect of applied bottom velocity direction, singled out and indicated by dashed-line squares in Figure 6.** The symbol "-" indicates that the direction is opposite to the reference model (Figure 3). **(a) Model melt fraction at the simulated end time (500 Myr),** blue line same as in Figure 3. **(b) The applied bottom horizontal velocity distribution,** **(c) model bottom dynamic topography** ( $h = \sigma_{rr} / [(\mathbf{g} \cdot \mathbf{n}) \cdot (\rho - \rho_{\text{core}})]$ , where  $\sigma_{rr}$  is the normal stress), **(d) model bottom melt fraction (left) and applied bottom temperature distribution (right)** ( $\Delta T = -200$  °K, Figure 6), **(e) the spatial distribution of the fixed melt fraction (0.16).** Dark blue model: The bottom horizontal velocity peak value ( $\Delta v$ , Figure 6) is 0.05 m/yr, and the velocity direction within the plume is away from the center (same as the reference model, Figure 3). Brown model: The velocity is 0.01m/yr, and the direction within the plume is towards to the center (opposite of the reference model). The melt morphology of the dark blue model is more consistent with the seismic constraints.

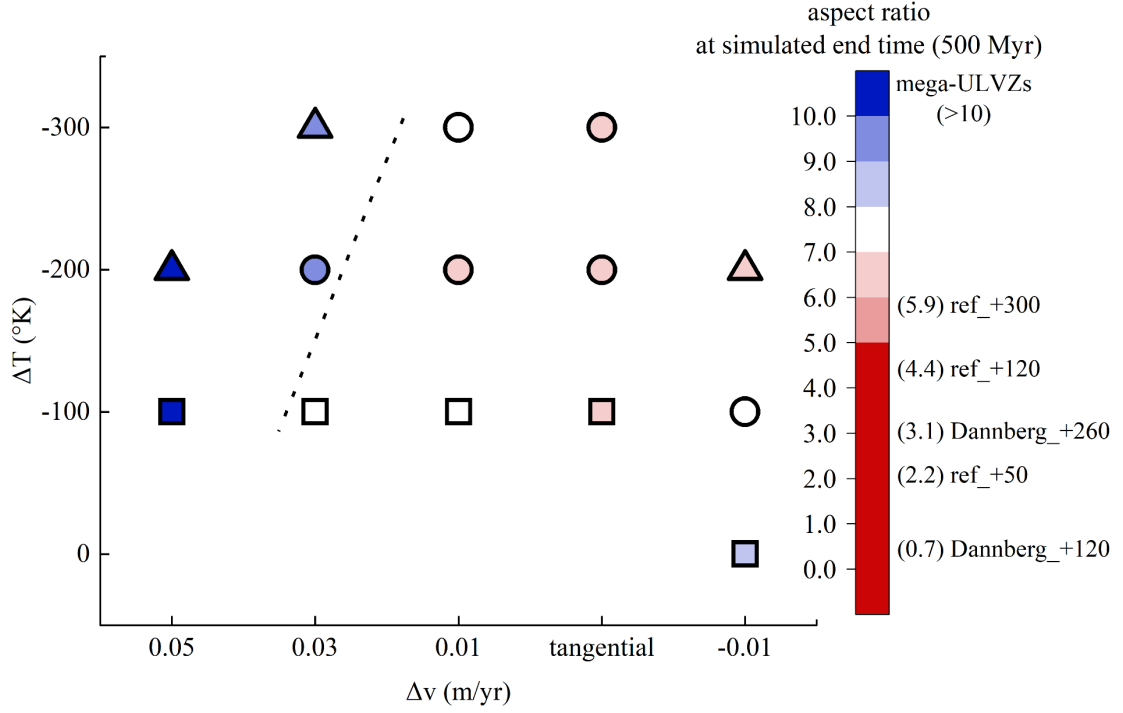
Figure 7a depicts the melt fraction distribution for both models at the end of the simulation (500 Myr). Figures 7b-d depict the results for the tangential velocity at the model's bottom boundary, the CMB dynamic topography, the melt fraction, and the applied temperature. Figure 7e's horizontal and vertical axes are spatial coordinates indicating the contour spatial distribution for melt fraction of 0.16. The dashed lines represent the location of ULVZ/plume edges.

The edge of the melt layer, where the mantle flow meets due to an abrupt change in velocity direction (Figure 7b), is the area of lower melt degree depicted in Figure 7a. However, compared to the smoother border of the negative model, the positive model's edge is steeper. The dynamic topography in Figure 7c similarly reflects this sharp edge; however, the negative model lacks this feature, whereas the positive model exhibits a local topographic jump with an amplitude of 1-2 km comparable to the total value. The melt fraction depicted in Figure 7d reduces toward the edges because of applied cold source temperatures and thermal diffusion. Particularly, the melt fraction in the model decreases by  $\sim 10\%$  within a few kilometers, corresponding to melt density variation and gradually increasing dynamic topography (Figure 7c). Finally, the melt fraction distribution (Figure 7a, e) shows that the positive model's lateral extent and aspect ratio of the melt layer are substantially larger, and the top region of its low melt fraction zone is flatter than that of the negative model.

More specifically, studies of long-wavelength topography demonstrate the contribution of LLVSP to lower mantle flow (Heyn et al., 2020; Lassak et al., 2010), and our results show that when the ULVZs are engaged, the topography undulations here are horizontally shorter ( $\sim 20$  km) and vertically more pronounced ( $\sim 1-2$  km). Previous studies estimated that a 1% melt corresponds to a shear wave velocity reduction of approximately  $\sim 2.5\%$  (Dannberg et al., 2021). Additionally, due to the cold source presence, there may be a "cooling zone" for the plume (with strong lateral heat flux), with a  $\sim 10\%$  lateral variation in shear wave velocity at the plume edge with a slightly lower melting degree. In summary, melt layer morphologies produced by models with bottom velocity in the same direction of the internal reverse circulation are

more consistent with the seismic observations (Rost et al., 2005). The local variation of the lateral melt fraction and the higher local topographic jump (gradient) at the plume edge are the main features of this model.

We then conduct a parameter analysis, as illustrated in Figure 8, to contrast the precise impacts of various model bottom conditions on the ULVZs morphology (aspect ratio).



**Figure 8. Phase diagram of melt aspect ratio for the models' bottom boundary setups.** The model density difference and plot symbols are the same as in Figure 6. *Aspect ratio* = (width / height)<sub>melt</sub>. *Melt width*: horizontal distance (left-side) from the model center to location where melt fraction contour (0.1) vertical-thickness reaches 5 km. *Melt height*: the height of the fixed melt fraction (0.1) in the model center. Colors indicate the melt aspect ratio at the simulated end time (500 Myr). The right-side legend symbols show the aspect ratio of the reference models (Figure 3) and the mega-ULVZs (Figure 1 and Table 1). The aspect ratios of the reference models are  $\leq 6$  (legend right), while all models with changed bottom boundary setup are  $> 6$  (background). The aspect ratios of top-left area models are more consistent with the seismic observational constraints.

As in Figure 6, the horizontal and vertical axes in Figure 8 represent the boundary conditions, and the symbols indicate whether the melt is stable. The color in the figure represents the melt aspect ratio at the end of the simulation. We take the height of the central melt fraction 0.1 as the ULVZ height, and the distance from the left fraction 0.1

up to 5 km thickness to the center as the ULVZ width. So, the aspect ratio is defined as melt width/melt height. Because the "Dannberg" model produces less melt, the melt fraction is set to 0.16, and the thickness limit is set at 1 km.

The reference model results (Figure 5) are also shown in the right of the legend. The melt aspect ratios of these bottom tangential flow models are  $<6$ , and the smaller the density difference, the lower the aspect ratio and the more "towering" the melt region, which is consistent with the results in Section 3.1. The models' aspect ratio with modified bottom condition are all  $>6$ , and the larger the velocity magnitude, the flatter the melt region in the positive model. It suggests that the stronger bottom tangential flow can suppress the wider range of mantle flow above the CMB, allowing the upper melt layer to have a greater lateral scope.

As mentioned in Table 1, the aspect ratio of the mega-ULVZs shown at the top of the legend is substantially bigger ( $>10$ ). Based on the thickness (5-40 km) and lateral extent ( $\times 10^2$ - $10^3$  km) of the ULVZs observed, the majority of the ULVZs can have  $>5$  aspect ratio. Therefore, if the simulation results are to be comparable with seismic observations, the high-density melt must be coupled to the bottom local CMB-mantle flow, where the flow velocity is in the same direction as the internal reverse circulation. Moreover, the magnitude of the flow velocity is related to the morphology of the melt.

#### **4.2.1 Other factors affecting the melt morphological characteristics**

In the previous sections, the applied cold source's peak value position—roughly 100 km from the mantle plume center—was fixed. First, we consider the impact of the cold source location on the melt chemical stability. We then adjust the distance from the peak value position of the applied cold source to the plume center, specifically, 50 km closer to and farther from the center. As a result, compared to the " $\Delta T_{200\_}\Delta v_{0.03}$ " model in Figure 5, the different models' melt growth rate: no cold source  $>$  cold source 50 km farther from the center  $>$  cold source -100 °K at the same position  $>$  cold source 50 km closer to the center  $>$  cold source -200 °K (" $\Delta T_{200\_}\Delta v_{0.03}$ ") (Figure S3). Observe that the cold source, both too close and too far from the plume center, increases the melt growth rate (unstable trend).

In terms of CMB dynamic topography, the distant cold source (+50 km) will mitigate the impacts of the local topographical undulation near the plume's edge. In contrast, a nearby cold source (-50 km) will just extend the lateral extent of the undulation, with minimal effect on the maximum topographical leap amplitude. In terms of melt morphology, the sharp-edged and flat-topped melt layer feature vanishes as the cold source advances farther from the mantle plume (+50 km). In contrast as the cold source approaches (-50 km), the smaller low-melting degree melt zones will emerge at the plume edge (Figure S4). The high-melting morphology at the bottom of the plume, however, is less affected by the nearby cold source.

As a result, the "cooling zone" for the plume must continue to be involved in the melt stabilization process. However, if the cold source is too close, it will change the low-melting morphology at the base of the plume, rising the two edges and severely lowering the center (Figure S4).

In addition, we investigated the impact of positive and negative Clapeyron-slopes on the " $\Delta T_{200\_}\Delta v_{0.03}$ " model results. We change the initial melt state parameters in Table 2 so that the melt layers in the positive slope model and the negative slope model are about the same thickness (~15 km) at the beginning of the modeling process (Table S1). The findings demonstrate that the negative Clapeyron-slope flattens the central low-melting zone but has no impact on the total melt-mass and melt growth rate at the simulated end time (Clapeyron-slope+:  $0.152 \text{ yr}^{-1}$ , Clapeyron-slope-:  $0.147 \text{ yr}^{-1}$ ) (Figure S5), nor does it have an impact on the dynamic topography at the CMB and the high-melting morphology on it (Figure S6).

### **4.3. The CMB dynamical environment implied by the ULVZs morphology**

Even further, based on the dynamic conditions of the previous sections, can we evaluate the characteristics of the bottom flow field from the ULVZs morphology? We previously applied a constant bottom velocity constraint, which is partly consistent with the morphological properties of the melt system once it reaches thermos-chemical-mechanical stability. In this section, the bottom tangential velocity is dynamically determined by the topographic horizontal gradient.



First, the bottom dynamic topography is calculated using the normal stress, specifically its perturbations with respect to the reference adiabatic-regime hydrostatic pressure,

$$\sigma_{rr} = \hat{g}^T \left( 2\eta \left( \varepsilon(\mathbf{u}) - \frac{1}{3} (\nabla \cdot \mathbf{u}) \mathbf{I} \right) \right) \hat{g} - p_d \quad (9)$$

where  $p_d = p - p_{\text{adiabatic}}$ ,  $\hat{g} = \frac{\mathbf{g}}{\|\mathbf{g}\|}$ .

The dynamic topographic is

$$h = \frac{\sigma_{rr}}{(\rho - \rho_{\text{core}})(\mathbf{g} \cdot \mathbf{n})} \quad (10)$$

where  $\rho_{\text{core}} = 9900 \text{ kg/m}^3$  (Dziewonski & Anderson, 1981).

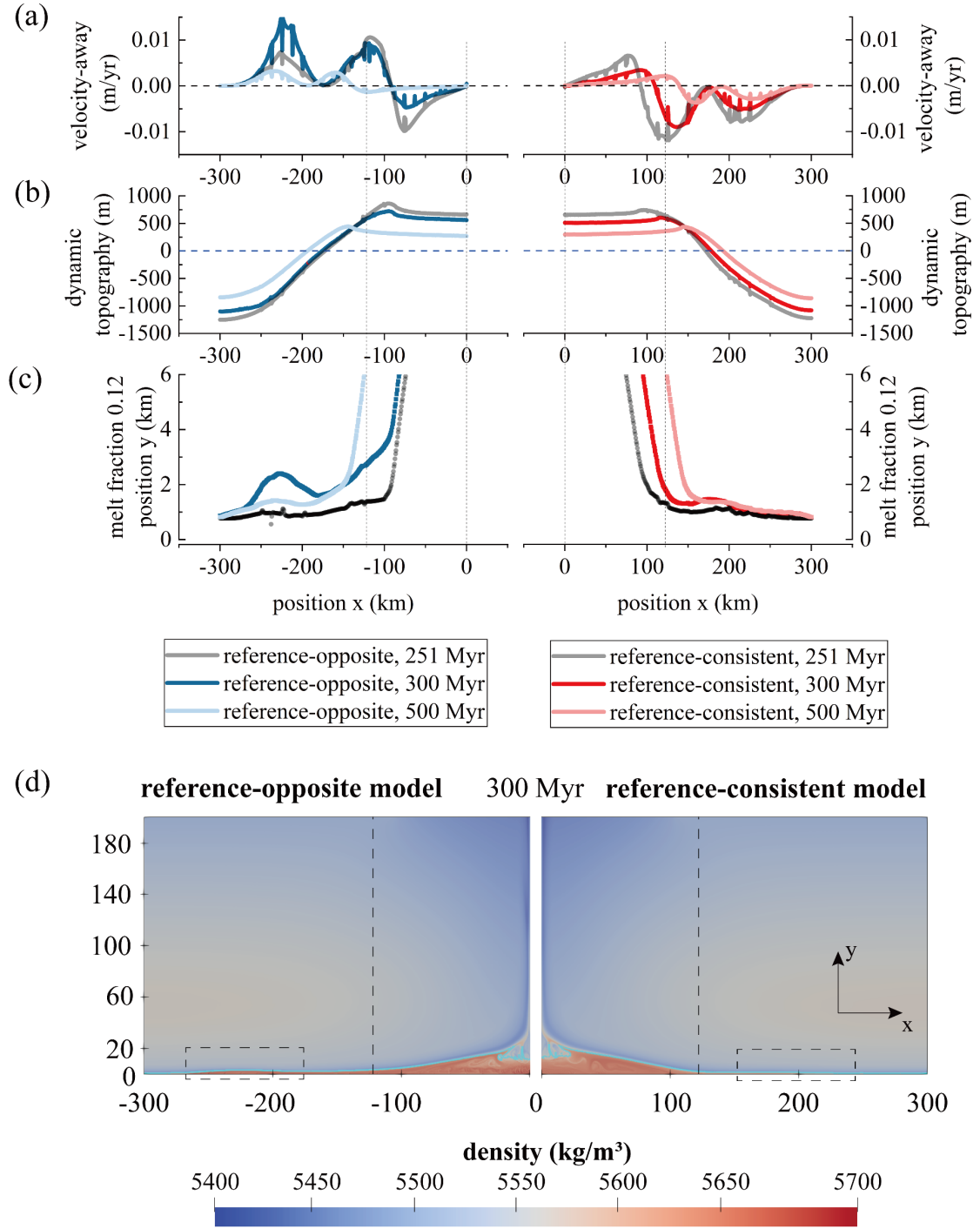
We refer to the equation used to calculate the normal infiltration rate in the "Lim" model (Lim et al., 2021), and here the topographic gradient is used to calculate the tangential velocity as

$$v = c \cdot \frac{\Delta\rho(\mathbf{g} \cdot \mathbf{n})}{12\eta} \cdot \nabla_x^2 h^4 \quad (11)$$

where  $c$  represents the dimensionless scaling factor.

We use  $\Delta T = 0 \text{ }^\circ\text{K}$ ,  $\Delta v < 0.02 \text{ m/yr}$  at the initial stage (250 Myr, consistent with the setup in Figure 4) because a greater " $\Delta v$ " results in numerical instability here. Due to the absence of cold source, the melted layer did not reach chemical stability. The results of the opposing horizontal velocity ( $x$ ) direction models are displayed in Figure 9, where "reference-consistent" indicates horizontal velocity  $x$  away from the center in the interior of the plume (consistent with the reference model in Figure 3), and "reference-opposite" indicates horizontal velocity  $x$  toward the center within the plume.

Specifically at the simulated end time (500 Myr), "reference-consistent" was slightly smaller (0.92) than the "ref\_+300" model, and "reference-opposite" was roughly equal to (1.00) the "ref\_+300" model. The generated melt layer has a lower aspect ratio as well. Here we mainly focus on the evolution and duration of some melt features.



**Figure 9. Model evolution results of topography-coupled bottom velocity boundary at 251 Myr (gray, the beginning of the setup), 300 Myr (dark color), and 500 Myr (light color). Reference-consistent:** red, horizontal velocity ( $x$ ) direction is applied away from the center within the plume, same with reference model (Figure 3). *Reference-opposite:* blue, horizontal velocity ( $x$ ) direction is applied toward the center within the plume. **(a) Bottom horizontal velocity ( $x$ ) distribution** ( $>0$ : away from the plume center,  $<0$ : towards the plume center), **(b) model bottom dynamic topography**, **(c) the spatial distribution of the fixed melt fraction (0.12).** **(d) The model mass-density at 300 Myr** (density  $\bar{\rho} = (1-\phi) \rho_{\text{solid}} + \phi \rho_{\text{melt}}$ ,  $\phi$  is melt fraction), the blue line is the same as in Figure 3. To reduce the disturbances of numerical errors,

for panels (a,b,c) and for each model we center on  $x = 0$  km and take averages (arithmetic mean) of the values of the variables from both sides about  $x=0$ ; then we plot them on the right side of the "reference-consistent" model and on the left side of the "reference-opposite" model respectively. (d) The black dashed-line boxes indicate a possible "melt bulge" area outside the plume in the "reference-opposite" model (left), virtually absent in the "reference-consistent" model.

Figure 9a represent the bottom tangential velocity ( $>0$ : away from the plume center,  $<0$ : towards the plume center) evolution, and the velocity at the side boundaries would still be artificially suppressed. In contrast to the previous model distribution, there are locations outside of the plume where the velocity drops to zero under the combined influence of topography and topographic gradient.

To reduce the influence of numerical errors, we center on vertical axis  $x = 0$  km, average the values on both sides (Figures 9a-c), and later for the figure plots we show the right side of "reference-consistent" and the left side of "reference-opposite" (Figure 9d). The results reveal that due to the larger topography gradient, the velocity near the plume edge (dashed vertical line) can be maintained for at least 50 Myr (250~300 Myr), while velocity values reduced in other areas. As for the later stage (300~500 Myr), the results demonstrate that the bottom velocity values rapidly rise at the locations of high strain rate, causing the melt layer to spread towards the outside of the plume (Figure 9d), leading to the local velocity within the plume to decrease (Figure 9a), the local topography to become smooth (Figure 9b), and the spatial distribution of the melt to increase (Figure 9c). We believe that (a) the lack of the cold source causes outward expansion of the melt layer with plume edge movement, and (b) bottom flow velocity with a simple constant scaling factor  $c$  in equation (11), both of which lead to the decay of the velocity magnitude within the plume at this stage.

Notably, the area away from the plume in the "reference-opposite" model (-250~-200 km in Figure 9c) forms the smaller "melt bulge". It should be noticed that even if we intentionally suppress the mantle velocity outside the plume, close to the side boundaries, the "melt bulge" still occurs. Finally, as the simulation progresses (300 Myr~500 Myr), the dynamic topography value decreases due to the continuous growth of the melt to both sides (Figure 9b), resulting in a decrease in the bottom velocity

magnitude (Figure 9a) and the height of the "melt bulge".

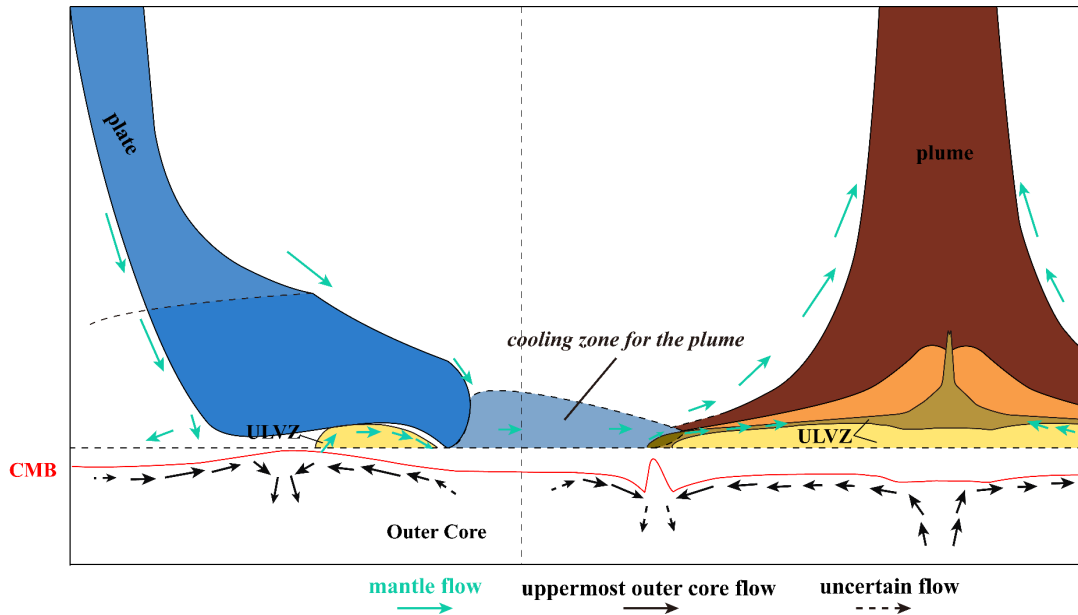
The "reference-consistent" modeling results partially indicate the dynamical environment around the hot mantle plume area, validating our "Dirichlet" boundary setup described in the previous sections. However, in order to understand the "reference-opposite" model findings, we must start with the conceptual model. The dynamical environments of the cold-downwelling zone and the ascending mantle plume are opposite, and under gravitational action, the opposite mantle flow produces the opposite CMB dynamic topography. Because the topographic gradients under these regions can be comparably strong and long-lasting here, CMB-mantle flow can be significantly influenced by uppermost core flow, and where the flow field direction may be opposite to that of regional mantle flow (Figure 10). Then a mantle "opposite" flow and corresponding boundary layer may exist over several kilometers of thickness, resulting in larger local viscous stress.

Therefore, the outer-plume region of the "reference-opposite" model may indicate the CMB-mantle flow near the cold zone, and the "melt-bulge" (found in the simulation) may correspond to the ULVZs in the cold zone. By suppressing the above-adjacent mantle flow near the cold-downwelling zone, the CMB-mantle flow (here in opposition) might, in theory, also contribute to the creation of the ULVZs. However, since the outer core cannot be properly recreated in our modeling, the "reference-opposite" model itself cannot provide robust evidence of the process, meaning a self-consistent mechanism for the generation of locally high stress that can contribute to the ULVZs development in cold zone.

Furthermore, how did the low-velocity material originate to form in the "cold zone"? Back to constant-in-time velocity model, which is applied with constant extended cold source ( $\Delta T = -100$  °K) and tangential velocity setup (as in the "reference-opposite" model,  $\Delta v = 0.01$  m/yr), the result shows that the similar appearance of "melt bulge" outside of the plume (Figure S7). The reduced melt fraction decreases the resulting melt-solid density difference, which reduces the CMB-mantle tangential flow velocity allowed by a gravitationally more stable structure. It ultimately lowers the length-scale and magnitude of "low wave-velocity anomaly". Our further validation of the low-

velocity material sources of partial melting in the cold zone is limited by the model's simplified material properties, such as linear solidus-liquidus. However, previous research indicates that the liquid core material can penetrate the CMB in the downwelling flow region, although the resulting "mushy layer" thickness is  $\sim 1$  km (Kanda & Stevenson, 2006; Lim et al., 2021). If the local CMB-mantle flow is involved, the initial formation melt will thicken into a "low-velocity zone", as shown in the model in this section. In general, due to limitations of the temperature and topographic gradient, the range of ULVZs developed here is narrower than that in the plume region, which may explain why some ULVZs and "low-velocity layer" appear in the "cold zone", as shown in Figure 1 (Fan et al., 2022; Yu & Garnero, 2018) (Figure 10). Compared to ULVZs formed near the superplume edge, ULVZs in the cold zone have a smaller scale and less lateral variation in seismic-wave velocity, which could be verifiable by geophysical observations.

Finally, we have discussed the mechanisms of melt stabilization at the plume edge and in the cold zone. However, the localized denser melts, detected by seismic observations at the bottom center of the plume, may not be "controlled" by the CMB-mantle flow due to small CMB-topographic gradients, and may continue to accumulate and grow until the lateral extent extends to a sufficiently cooled zone, where P-T conditions will limit the amount of melt and preclude further melt growth-advancement, by melt-solid equilibration. From our reference modeling results (Figure 5 and 8), during this process, compared to plume edge ULVZs, larger melt heights and smoother-edge ULVZs morphology are probably its main characteristics.



**Figure 10. Schematic representation of the model conclusions.** The subdomain on the right side from the vertical dashed line indicates the study area involved in our model, and the left side indicates the presumed environment involved in the cold downwelling. Note the near-bottom dashed horizontal line is a simple referential CMB, which the **red solid line** depicts a dynamic CMB responding to this plume-and-plate environment. **Dark brown:** the mantle plume, **orange tones:** the melting layer with increasing melt degrees (darker), **blue:** the cold subduction plate (solid line), and the high-velocity layer of the resulting cold source (dashed line). The melt fraction is lower at the area where the "cooling zone" meets the edge of the plume. **Yellow:** The ULVZs, occur at the plume's base and in areas with large CMB topographic gradients of the "cold zone". **Cyan arrows:** the lowermost mantle flow direction, **black solid arrows:** the flow direction near the CMB and at the uppermost outer core, **black dashed arrows:** the core flow with assumed direction.

#### 4.4. Model limitations

Our model is simplified by using a 2D geometrical description, also by having a constant distribution coefficient of Fe, Mg between the solid and liquid phases, as well as a linear solidus-liquidus equation curve. It was chosen to isolate the effect of bottom boundary conditions on melt generation and to speed up simulations for comparing different model setups. This simplification may lead to some inaccuracies related to the following:

(1) Compared to a 3D model, the 2D model we introduced neglects heat transfers in the 3<sup>rd</sup> direction and thus probably underestimates the plume heat losses. And 2D Dirichlet velocity BC would require mostly exaggerated drag forces on the CMB to

generate the tangential velocity consistent with the magnitude of the lowermost mantle flow.

(2) Compared to the "Dannberg" model, the material properties we used exaggerate the total melt mass; to avoid this, we focus on the melt growth rate and the aspect ratio of melt morphology.

(3) We did not explore the effect of viscosity. Still, previous studies indicated that the height of ULVZ is not sensitive to its viscosity (Beuchert & Schmeling, 2013), and whether viscosity affects the melt morphology in the edge area requires further study.

(4) We did not directly/explicitly model the mechanical interaction between subducting plates and ambient mantle, nor the intercoupling between the subducting plates and the low-viscosity outer core; due to numerical stability limitations and to isolate the basic controlling factors conveniently; instead, we applied different bottom boundary conditions at a certain time, which led to the resulting evolution of the ULVZs differing slightly from the corresponding geological evolution of the real Earth.

In order to stay focused on the specific problem, most discussions in this study are based on our numerical models, which are symmetric about  $x = 0$ . In further studies, different scales, extents and locations of cold sources and/or CMB-mantle flows might be considered, and purposely applied to the left or the right side, in order to examine asymmetric scenarios that are closer to the real Earth.

## 5. Conclusions

(1) The stable existence and residence of high-density ( $(\rho_{melt}-\rho_{solid})/\rho_{solid} > +1\sim 2\%$ , even up to  $\sim +10\%$ ) melt requires, in the scenario we studied, the participation of a cold source, and corresponding lateral temperature differences between  $\sim 4000$  °K at the plume central regions to  $< \sim 3900$  °K at the plume-cooling intermediate mantle region, separated by horizontal distances of about 100 ( $< \pm 50$ ) km. The plume-cooling intermediate region is the region where heat flows from the hot plume base (at the center of our model) towards a neighboring cold-source (not explicitly modeled in our settings) such as a subducted plate that advected cold isotherms from the surface (Figure 10); a configuration that may last for several hundred Myr regarding mantle viscosities and thermal diffusivities.

(2) To obtain the ULVZs results with a high aspect ratio that matches seismic observations, the high-density melt requires the participation of a CMB-mantle flow that is oriented with internal reverse circulation of/inside the plume broad basal region. Furthermore, the fluid dynamics of this problem dictates that the solid velocity magnitude is related to the melt liquid-body morphology. ULVZs morphology with a flat top and sharp edge necessitate local CMB-mantle flow horizontal speeds about  $>3$  times the characteristic convective speed of the lower mantle ( $\sim 1$  cm/yr), and this could be attained by episodic mantle forces and/or outer core interactions (favored by CMB topography that enhances resistance and coupling of the flow stresses, and potentially/eventually magnetic forces).

(3) The local CMB-mantle flow facilitated by CMB topography interacting with the outer core may be important (and perhaps crucial) in developing mega-ULVZs, especially when the latter is spread/located near the edges of a superplume; phenomena which may be transient in the Earth's mantle evolution. Our point of view is related to the fact that seismic-observations studies discovered ULVZs in some "cold zones" with higher seismic-wave speeds. Still, their lateral extents are smaller due to temperature and topographic gradient amplitude limitations.

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## **Data Availability Statement**

Our modeling results, ASPECT input file and plugin are available at (<https://zenodo.org/records/10006400>). Version 2.4.0 of the numerical software ASPECT



used for modeling is available via <https://zenodo.org/record/6903424>, the visualization software ParaView is available via <https://www.paraview.org/>. Figure 1 is plotted with GMT <https://www.generic-mapping-tools.org/>.

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