# Contrasts in two- and three-dimensional system behaviour in the modelling of compositionally originating LLSVPs and a mantle featuring dynamically obtained plates

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# <sup>10</sup> Running Title:

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## <sup>11</sup> Modelling LLSVPs and plates in mantle convection models

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**SUMMARY** More than two decades of systematic investigation has made steady progress 12 towards generating plate-like surface behaviour in models of vigorous mantle convection. Ac-13 cordingly, properties required to obtain dynamic plates from mantle convection have become 14 widely recognized and employed in both 2D and 3D geometries. Improving our understand-15 ing of the properties required to obtain durable (or replenishable) deep mantle features with 16 LLSVP-like characteristics has received interest for a period with similar longevity. Inves-17 tigation ultimately focusses on discovering the properties able to produce the presence of 18 a detached pair of three-dimensional features, distinct from the ambient mantle. Here, we 19 assume the LLSVPs have a chemical origin by incorporating a Compositionally Anomalous 20 and Intrinsically Dense (CAID) mantle component comprising 2-3.5% of the total mantle 21 volume. The feedback between plate formation and the presence of a CAID mantle compo-22 nent is investigated in both 2D and 3D spherical geometries. We explore the impact of both 23 an intrinsic contrast in density and viscosity for the CAID component, with the objective 24 of finding system parameter values that encourage the formation of a pair of LLSVP-like 25 assemblages and a surface that exhibits the principle features of terrestrial plate tectonics; 26 including recognizable and narrowly focussed divergent, convergent and (in 3D) transform 27 plate boundaries that separate 8-16 distinct plate interiors. We present the results of nine 28 two-dimensional and eleven three-dimensional calculations and show that for some of the 29 cases examined, a pair of CAID material provinces can be freely obtained in two-dimensional 30 cases while maintaining a surface characterized by plate-like behaviour. However, specifying 31 the same system parameters in the three-dimensional model does not readily yield a pair of 32 enduring provinces for any values of the parameters investigated. Moreover, the inclusion 33 of the CAID component in the mantle can affect the global geotherm so that in comparison 34 to the surface behaviour obtained for the initial condition isochemical model, the surface 35 behaviour of the cases incorporating the dense component are less exemplary of plate tecton-36 ics. In general, CAID material components that are 3.75%-5% denser than the surrounding 37 mantle (at surface temperatures), and up to a factor of 100 times greater in intrinsic vis-38 cosity, form layers populated by voids, or nodes connected by tendril-like ridges that reach 39 across the core-mantle-boundary, rather than distinct piles resembling LLSVPs. Due to its 40 inherently heavy and stiff character, in equilibrated systems, we find the CAID material 41 becomes especially hot so that the temperature-dependence of its density and viscosity re-42 sults in reduced distinction between the intrinsically dense assemblages and the ambient 43 mantle. Accordingly, the CAID material forms masses on the CMB that are relatively less 44

dense (0.625%-1.5%) and viscous than the adjacent mantle material, in comparison to the
percentage differences obtained at common temperatures. We find that by adjusting our
yield stress model to account for the influence of the CAID material on the geotherm, a
highly satisfactory plate-like surface can be re-attained, however, the formation of a pair of
LLSVP-shaped masses remains elusive.

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#### <sup>53</sup> 1 Introduction

The Large Low Shear-wave Velocity Provinces (LLSVPs) observed below Africa and 54 the Pacific Ocean (Ritsema et al., 1998; Ni et al., 2002; To et al., 2005; Garnero & Mc-55 Namara, 2008; Hernlund & Houser, 2008; Auer et al., 2014) comprise first order physical 56 features in the lower mantle. Evidence that supports an at least partial chemical origin for 57 the LLSVPs includes seismic observations of broadly spanning velocity-magnitude anomalies 58 and the sharp shear-wave velocity gradient boundaries that confine these regions (Ritsema 59 et al., 1998; Ni et al., 2002; To et al., 2005; Garnero & McNamara, 2008; Lekic et al., 60 2012). However, the inferred densities of the volumes encompassed within the LLSVPs 61 vary. Evidence from the analysis of solid Earth tides (Lau et al., 2017) permits density 62 anomaly excess of little more than a half percent in the LLSVPs, relative to the adjacent 63 mantle. The Stonely modes of free oscillation data (Koelemeijer et al., 2017) suggest that 64 the provinces are less dense overall than the surrounding mantle, despite their deep location. 65 Such findings may hint at LLSVP evolution that is consistent with marginally stable, chem-66 ically dense but relatively hot, transient sluggish masses (Li et al., 2019) rising from the core 67 mantle boundary (CMB). In any case, the conflicting observations add to the uncertainty 68 in resolving the physical parameters responsible for the LLSVPs (e.g., McNamara, 2019). 69 Indeed, several studies have shown that the morphology of the seismically slow provinces 70 might be explained by thermal anomalies in isochemical models (Schuberth et al., 2009, 71 2012; Davies et al., 2015). However, although arguments for purely thermal origins for 72 the LLSVPs are credible, the observation of an anticorrelation between bulk sound and 73 shear modulus (Su & Dziewonski, 1997; Ishii & Tromp, 1999; Masters et al., 2000; Tram-74 pert et al., 2004; Moulik & Ekström, 2016) makes a compositional origin for the LLSVPs 75

a compelling hypothesis. Accordingly, thermochemical modelling of the evolution of the
deep mantle requires obtaining discrete compositionally originating piles on the CMB that
spend at least part of their existence coalesced into a pair of roughly diametrically opposed,
steep-sided, hot but intrinsically dense provinces. Moreover, the detached chemically distinct volumes comprising the piles may reach over a thousand kilometres in height above
the CMB (Cottaar & Lekic, 2016).

The longevity of this arrangement may exceed several mantle transit times (the time 82 required for a parcel of mantle material to traverse the depth of the mantle at the mean 83 velocity of the plates). Previous studies have concluded that the LLSVPs have occupied 84 their current positions for several hundred million years (Burke & Torsvik, 2004; Dziewonski 85 et al., 2010; Torsvik et al., 2010). The location of large igneous provinces (LIPs) suggests 86 a correlation with the peripheries of the LLSVPs which have been argued to be the site 87 of plume generation zones (PGZs) formed by the influence of a sharp lateral temperature 88 gradient at the edges of thermochemical provinces (Torsvik et al., 2006; Burke et al., 2008; 89 Li & Zhong, 2017; Heyn et al., 2020). Given this connection, the age and positioning of the 90 LIPs suggests that the LLSVPs are both stable and relatively immobile (at least some of the 91 time) for periods in excess of 200 Myr. However, intermittent mobility of the LLSVPs, as well 92 as changes in their morphology, in response to plate motion and subduction zone migration 93 is evident in thermochemical convection studies that have imposed plate reconstruction 94 histories as surface boundary conditions (McNamara & Zhong, 2005; Zhang et al., 2010; 95 Flament et al., 2017). These studies have incorporated intrinsically dense components that 96 produce a pair of LLSVP-configuration provinces in response to the imposition of an evolving 97 plate velocity field that agrees with inferred records for the past 200+ Myr and speculative 98 histories extending back hundreds of millions of years before that. Although two current-99 day LLSVP-type thermochemical features can be obtained on the CMB when recent plate 100 history is simulated, it is not clear that broad chemically distinct provinces on the CMB 101 can be obtained when full feedback between a thermochemical mantle component and the 102 plates is modelled. 103

Adhering to the hypothesis that the LLSVPs are compositional in nature (Humayun et al., 2004; Tackley et al., 2005; Boyet & Carlson, 2006; Labrosse et al., 2007; Deschamps et al., 2011), we investigate the feedback between a dynamically evolving plate-like surface velocity field in two- and three-dimensional thermochemical mantle convection models and the distribution of a compositionally anomalous and intrinsically dense (CAID) component

introduced into the deep mantle of vigorously convecting systems (e.g., Trim et al., 2014; 109 Trim & Lowman, 2016; Stein et al., 2020). With plates being absent, previous findings 110 (e.g., Hansen & Yuen, 1989; Tackley, 1998; LeBars & Devaille, 2004; McNamara & Zhong, 111 2004; Li et al., 2014; Tan et al., 2011) demonstrated the ability of a compositionally dense 112 mantle component to aggregate into a small number of stable piles that may interact with 113 the ambient mantle by responding to downwelling flow or influencing upwelling location. 114 The primary controlling influence over pile durability and longevity is the contrast in den-115 sity between the ambient and enriched mantle. In addition, pile stability and morphology 116 117 has been shown to be dependent on the thermally derived viscosity contrast within the convecting system (Li et al., 2014) as well as the intrinsic viscosity contrast between the 118 ambient mantle and CAID material (McNamara & Zhong, 2004; Heyn et al., 2018). The 119 rheological properties of a compositionally distinct component comprising the LLSVPs is 120 not known but it has been proposed that the LLSVPs are either enriched in Bridgmanite 121 and iron (Trampert et al., 2004) or depleted of ferropericlase (Yamazaki & Karato, 2001). 122 Given that an absence of interconnected regions of lower viscosity ferropericlase would have 123 a lower viscosity than a nearly pure Bridgmanite component (Ballmer et al., 2017), it may be 124 that the LLSVPs are inherently more viscous than the material in the surrounding mantle. 125

Due to feedback, the simultaneous modelling of dynamically obtained plates and an 126 intrinsically dense component in the deep mantle is a problem that is distinct from the mod-127 elling of either a system that features compositionally dense piles while lacking plates or 128 the obtaining of a plate-like surface over-lying an interior where dense provinces are absent. 129 For example, previous studies have shown that, when they form, dense piles become mobile 130 or susceptible to breakup as a result of the impact of slab-like downwellings (Hansen and 131 Yuen, 1989; McNamara & Zhong, 2005; Langemeyer et al., 2020). Plate-like surface char-132 acteristics produce especially focussed sheet-like downwellings and can also have a strong 133 effect on heat flow and the temperature profile of the mantle (Lowman et al., 2001); poten-134 tially changing the requirements for pile formation. Similarly, the presence of compositional 135 provinces influences heat flow (Amit & Olson, 2015; Li et al., 2018; Langemeyer et al., 2020) 136 at the core mantle boundary (CMB), altering the thermal profile of the system and there-137 fore a property upon which the obtaining of a plate-like surface behaviour strongly depends 138 (e.g., Stein & Hansen, 2008). Accordingly, the addition of a CAID component to a mantle 139 convection model exhibiting self-consistently generated plates can, potentially, result in the 140 cessation of the plate behaviour (Trim et al., 2014). Moreover, LLSVP-emulating provinces 141

can influence the positioning of thermal plumes which, in turn, can disrupt the stability of 142 the plates and the quiescence of their interiors. However, the converse is similarly applica-143 ble. The inclusion of CAID material in the convecting system has the potential to be the 144 ingredient that alters the thermal field in a way that can allow plates to form when other 145 system parameters would otherwise not be conducive to their generation. Determining the 146 physical requirements for the generation of plates and LLSVP-like compositionally origi-147 nating provinces is thus a problem that simultaneously requires satisfying two requirements 148 influenced by the same parameters. 149

Recognizing that the existence of plate tectonics and the LLSVPs are distinct but 150 coupled features simultaneously required by a global mantle convection model presents con-151 straints and the potential for discovering limits on the composition of the LLSVPs. A small 152 number of studies of the dynamic interaction between these two first-order features at the 153 surface and base of the mantle have been presented (Trim et al., 2014; 2016) but continued 154 investigation may provide important further insight into important physical mechanisms 155 governing the Earth's evolution. For example, two-dimensional modelling has shown that 156 the formation of a pair of CAID material provinces with LLSVP-type morphologies is not 157 guaranteed by the inclusion of a dense component in a fully dynamic model, but that 158 two stable, non-transient, piles can be obtained if the CAID material has specific qualities 159 (Langemeyer et al., 2018, 2020; Li et al., 2019). Previous studies (Trim et al., 2016) have 160 also shown that when a small number (1-3) of durable provinces are obtained, they can be 161 as mobile on the CMB as continents on the surface. Understanding whether CAID material 162 provinces are inherently stationary or prone to episodic bouts of translation also requires 163 modelling in conjunction with the existence of dynamic plates. 164

In this study we further investigate the feasibility of and requirements for distributing 165 a compositionally anomalous component of the mantle into two distinct and detached large 166 provinces. Previous work employing two-dimensional calculations (Langemeyer et al., 2020) 167 showed that in systems featuring self-consistently evolving plates, the formation of a small 168 number (i.e., 1-3) of provinces was just one possible outcome for the distribution of a dense 169 component comprising between 3 and 5% of the mantle's volume. Following the examples 170 of previous studies, these authors varied both the relative intrinsic density and viscosity of 171 the dense mantle component (e.g., Heyn et al., 2018; Li et al, 2014; Deschamps & Tackley, 172 2008) and found that specific combinations of these parameters were conducive to producing 173 a durable and persistent pair of provinces that yielded periods in which LLSVP-like topo-174

graphic profiles were obtained. (Alternative formations of the dense components range from a basal layer to multiple lower-volume piles.) In this study, we continue the approach of the previous work by first examining the influence of the stress-dependence of the lithosphere's rheology on the formation of the plate boundaries and the distribution of the CAID material in two-dimensional calculations and, subsequently, we model full 3D spherical shell systems featuring evolving plates and an intrinsically dense component.

181 2 Methods

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# 2.1 Governing Equations

Thermochemical convection is modelled in a spherical geometry using a finite volume code (Tackley, 2000) for solving the dimensionless equations of mass, momentum and energy conservation in a bi-modally heated infinite Prandtl number Boussinesq fluid. Advection of the compositional field is calculated using the tracer-ratio method (Tackley & King, 2003). Thus, we specify

$$\nabla \cdot \mathbf{u} = 0 \tag{1}$$

$$\nabla \cdot [\eta (\nabla \mathbf{u} + (\nabla \mathbf{u})^T)] - \nabla P = (-\mathrm{Ra}_{\mathrm{T}}T + \mathrm{Ra}_{\mathrm{c}}C)\hat{r}$$
<sup>(2)</sup>

$$\frac{\partial T}{\partial t} = \nabla^2 T - \mathbf{u} \cdot \nabla T + \mathbf{H}$$
(3)

188 and

$$\frac{\partial C}{\partial t} = -\mathbf{u} \cdot \nabla C \tag{4}$$

where **u** is velocity,  $\eta$  is dynamic viscosity, P is the non-hydrostatic pressure, T is temperature, t is time, H is the non-dimensional internal heating rate, Ra<sub>T</sub> is the reference thermal Rayleigh number, Ra<sub>C</sub> is the compositional Rayleigh number and C is the compositional field. The compositional field tracks the distribution of the intrinsically dense material such that  $0 \le C \le 1$  and the value of C gives the ratio of the mass of the CAID material to the total mass, per unit volume. A region featuring a compositional value of C = 1 is entirely comprised of enriched material, while C = 0 represents the ambient mantle. Equations (1) - (4) have been non-dimensionalised utilizing a thermal diffusion timescale. Furthermore,  $\eta = \bar{\eta}/\eta^*$ , where  $\bar{\eta}$  is the dimensional field and  $\eta^*$  is the dimensional reference viscosity.

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The thermal Rayleigh number and compositional Rayleigh number are defined as:

$$Ra_{T} = \frac{\rho_{0}g\alpha\Delta Td^{3}}{\kappa\eta^{*}}$$
(5)

199 and

$$Ra_{C} = \frac{\Delta \rho_{C} g d^{3}}{\kappa \eta^{*}},\tag{6}$$

where  $\rho_0$  is the reference density defined as  $\rho_0 = \rho(T_0)$ ,  $\alpha$  is the thermal expansivity, d is the thickness of the mantle,  $\Delta T = T_b - T_0$  is the difference between the superadiabatic isothermal basal temperature  $(T_b)$  and the isothermal surface temperature  $(T_0)$ , g is acceleration due to gravity,  $\Delta \rho_C$  is the contrast in density between intrinsically dense and ambient mantle material and  $\kappa$  is the thermal diffusivity.

The contrast in the Rayleigh numbers is described by the value of the buoyancy number  $B = Ra_C/Ra_T = \Delta \rho_C/(\rho_0 \alpha \Delta T)$  (representing the relative influence of thermal and compositional effects on the density of the mantle material). For example, with a buoyancy number of 0.5 the Boussinesq approximation results in an enriched mantle component at a non-dimensional temperature of 0.5 having the same density as the ambient mantle at a non-dimensional temperature of 0.0. (In general, for constant thermal expansion coefficient,  $\rho(T = B, C = 1.0) = \rho(T = 0.0, C = 0.0)$ ).

The governing equations (1) - (4) are thus completed by the incorporation of a linearized equation of state

$$\rho(T,C) = \rho_0 [1 + \alpha \Delta T (BC - T)]. \tag{7}$$

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The non-dimensional internal heating rate is defined as:

$$H = \frac{\rho_0 \epsilon d^2}{k \Delta T} \tag{8}$$

Quantity	Dimensional Value
$\eta^*$	$4.5 \times 10^{19} \text{ Pa} \cdot \text{s}$
$\kappa$	$1 \times 10^{-6} \text{ m}^2 \text{ s}^{-1}$
d	$2.89\times 10^6~{\rm m}$
$\Delta T$	$2500 \mathrm{K}$
diffusion time, $d^2/\kappa$	$265 { m ~Gyr}$
$ ho_0$	$3700 {\rm ~kg} {\rm ~m}^{-3}$
g	$10 \mathrm{~m~s^{-2}}$
$\alpha$	$2 \times 10^{-5} \ {\rm K}^{-1}$
k	$4.3 \text{ W m}^{-1} \text{ K}^{-1}$

 Table 1. Dimensional quantities adopted for this study.

where  $\epsilon$  is the dimensional heating rate per unit mass (specified here as uniform throughout the mantle) and k is the thermal conductivity. The dimensional values corresponding to the reference Rayleigh number and assumed in the dimensional interpretation of the results are provided in Table 1.

219 2.2 Rheology

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A mobile surface is attained through the implementation of a temperature-dependent viscosity combined with viscoplastic yielding. The viscosity temperature-dependence is specified using a non-dimensional Arrhenius-type law, where

$$\eta_T = \exp\left(\frac{E_a}{T+1} - \frac{E_a}{2}\right) \tag{9}$$

where  $E_a$  is a non-dimensional activation energy, determining the magnitude of the viscosity contrast due to temperature alone, between material at the surface and the core mantle boundary (CMB). This study uses a set value of  $E_a = 29.96$  to generate a thermal viscosity contrast,  $\Delta T$ , of  $3.2 \times 10^6$ .

A non-dimensional yield stress,  $\sigma_{\text{yield}}$ , is implemented by prescribing a surface yield stress value,  $\sigma_{\text{surf}}$ , and a mantle yield stress value,  $\sigma_{mantle}$ , that defines the yielding point below a prescribed non-dimensional depth,  $d_l$ . The prescribed depth-dependent yield stress is

$$\sigma_{\text{yield}} = \min[\sigma_{\text{mantle}}, \sigma_{\text{surf}} + \frac{D(\sigma_{\text{mantle}} - \sigma_{\text{surf}})}{d_l}], \tag{10}$$

where D is a non-dimensional depth below the model surface and  $d_l$  is the depth below which the mantle is prescribed a fixed yield stress value of  $\sigma_{mantle}$ .

We incorporate plastic yielding by utilizing a linearly proportional relationship between
 yield stress and yield viscosity, such that

$$\eta_{\text{yield}} = \frac{\sigma_{\text{yield}}}{2\dot{\epsilon}} \tag{11}$$

where  $\dot{\epsilon}$  is the second invariant of the strain rate tensor,  $\sqrt{\frac{1}{2}\dot{\epsilon_{ij}}\dot{\epsilon_{ij}}}$ .

In addition to the influences of temperature and stress, the variation in the rheological behaviour of the system is augmented by the inclusion of a specified increase in lower mantle viscosity. A number of geophysical observables have inferred an increase in mantle viscosity by a factor of 30 or greater at a depth corresponding to the phase transition from spinel to Bridgmanite + magnesiowüstite (Boehler, 2000; Hager, 1984; Richards & Hager, 1984; King & Masters, 1992; Mitrovica & Forte, 2004). Therefore, we specify an increase in lower mantle viscosity so that

$$\eta_{\rm TD} = \eta_{\rm T} \times \eta_{\rm D},\tag{12}$$

243 where

$$\eta_{\rm D} = 1 \quad \text{for} \quad z \ge 1 - 0.227 \quad \text{and} \quad \eta_D = 30 \quad \text{for} \quad z \le 1 - 0.227,$$
(13)

where z represents the non-dimensional height above the core mantle boundary with z = 1 - 0.227 corresponding to a dimensional depth of 660km.

To account for the impact on viscosity of temperature, depth and stress dependence, we define a composite viscosity that considers the relative importance of the contributing influences

$$\eta_{\rm comp} = 1/[1/\eta_{\rm TD} + 1/\eta_{\rm yield}].$$
 (14)

The final effect on viscosity, specifically explored in this study, is the specification of an intrinsic viscosity contrast owing to composition,  $\Delta \eta_c$ . The two component fluid has a viscosity given by  $\eta_{\text{comp}} \times (\Delta \eta_c)^C$ , where C is the local value of the composition field.

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## 2.3 Thermal steadiness

In this study, we vary  $\Delta \eta_c$ , the buoyancy number, B, the yield-stress value as a func-253 tion of depth and the volume of the intrinsically dense component in the systems. All cases 254 featuring a CAID material component are initiated from snapshots taken from statistically 255 steady systems that feature no CAID component. Details of the initial conditions are given 256 in the following section. The calculations incorporating CAID material are each a continu-257 ation of the calculation used to obtain the initial condition, with the addition of a uniform 258 thickness layer of CAID material enveloping the core at the start of the new experiment. 259 Subsequently, these new systems converge to statistically steady states themselves. 260

Calculations are considered to have reached a statistically steady-state when heat flow from the surface is balanced by the sum of the heat flow from the core to the mantle and the internally generated heat. Specifically, a steady-state is considered to be established when the time-averaged non-dimensional internal heating rate (set to 30 in all calculations) is equal to the difference in non-dimensional heat flows:

$$\frac{3(F_s - F_b f^2)}{1 + f + f^2},\tag{15}$$

where  $F_s$  and  $F_b$  are the mean non-dimensional surface and basal heat fluxes and f is the ratio of core to planetary radius (we specify a terrestrial value of 0.547 in this study). Convergence to a temporally averaged steady-state condition is obtained for the initial condition used in both the 2D and 3D calculations.

#### 270 3 Results

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## 3.1 Yield stress and model dimension

We first consider the behaviour of two-dimensional systems with a uniform nondimensional yield stress of  $2 \times 10^7$  (110 MPa). Previously, Langemeyer et al. (2020) described

the evolution of two-dimensional calculations featuring a yield stress of  $1 \times 10^7$  in other-274 wise identical systems. However, employing the same values for the system parameters, 275 Langemeyer et al. (2021) showed that in isochemical three-dimensional systems, a uniform 276 yield stress of  $2 \times 10^7$  results in a more plate-like surface behaviour, with time-dependent 277 boundaries that commonly exhibit Earth-like structure; namely, the appearance of spread-278 ing boundaries comprised of divergent segments and transform-like offsets coexisting with 279 contrasting arcuate convergent boundaries. The primary objective of the study presented 280 here is to examine the feedback between plate-like surface behaviour and a CAID compo-281 nent in the lower mantle, and to gain insight into any differences arising from the system 282 dimensionality. Accordingly, we employ the higher yield stress in all calculations by first 283 re-examining the behaviour of 2D systems. In later sections we present 3D calculations 284 featuring a CAID component with other system parameter values matching those employed 285 by Langemeyer et al. (2021). 286

The impact of the higher yield stress is to reduce the number of surface weak zones associated with subduction and divergence. The distribution of CAID material and the internal thermal structure are affected. As in the previous two-dimensional modelling work (Langemeyer et al., 2020) the buoyancy number of the CAID material as well as its viscosity relative to the ambient material are both varied, in order to determine their influence on the distribution of the CAID material.

We introduce a naming convention to simplify the discussion. Model names follow the format #DBbbDdd, where bb is the buoyancy number of the intrinsically dense material, dd is the contrast in viscosity between ambient and intrinsically dense material (at the same temperature and depth), represented as a multiplicative factor, and # is the number of dimensions used in the calculation. For example a three-dimensional calculation featuring a buoyancy number of 0.85 and a CAID material intrinsic viscosity that is a factor of 10 times greater than the viscosity of the ambient mantle material is designated: Model 3DB0.85D10.

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#### 3.2 Initial condition

Figure 1 shows the initial condition fields used for all 2D calculations presented. Corresponding temperature and viscosity are shown and reveal a pair of distinct downwellings. The initial condition is generated using an isochemical model. The surface features spreading centres and downwelling generating zones of focussed plate convergence, while the base



Figure 1. The initial condition non-dimensional temperature and viscosity fields used for all 2D calculations presented in this study. All two-dimensional calculations presented are obtained for a spherical annulus geometry with a resolution of  $128 \times 1024$ . The CAID material advection is modelled with the tracer ratio method (Tackley & King, 2003) using approximately 4.2 million tracers in each case.

of the mantle produces multiple active upwellings. The 2D calculations presented in the remainder of this study are initiated by adding a uniform height layer of CAID material enveloping the CMB, into the fields shown in Fig. 1. The evolution of this material is then analysed with time 0.0 corresponding to the initial condition.

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#### 3.3 Distribution of the CAID material in 2D calculations

Figure 2 shows temperature and composition field snapshots from nine calculations in which all parameters are identical, with the exception of the buoyancy number of the CAID material and its viscosity relative to the ambient mantle ( $\Delta \eta_C$ ). The CAID material comprises 3.5% of the mantle volume in all calculations. The snapshots show the presence of either one or two downwellings that are formed by surface convergence at a high-stress originating weak zone. In general, these downwellings persist for approximately one to several mantle transit times before waning. Upwellings forming in regions devoid of CAID material, as well as on top of CAID provinces, lack the vigour to reach the base of the plates. For cases where  $\Delta \eta_c = 1$  or 10, upwellings commonly occur at the edges or highest elevation points of the dense provinces. In cases where  $\Delta \eta_c = 100$  upwelling formation is often coincident with the points of highest elevation above CAID material piles. Regardless of the location of upwelling formation, at no point are upwellings observed to impinge upon the lower lithosphere.

Throughout the evolution of these calculations the intrinsically denser component is 323 often distributed into one large pile with intermittent episodes characterized by the forma-324 tion of two piles (often diametrically opposed). The cases shown exhibit a single pile (with 325 small secondary piles in some cases) when  $\Delta \eta_c \geq 10$  or 100. In contrast, two diametrically 326 opposed piles are common when  $\Delta \eta_c = 1$ . We also find that a pair of diametrically opposed 327 piles of similar size are often present early in model evolution (e.g., in Models 2DB0.75D100 328 and 2DB1.0D100), but eventually a single pile is formed. In general, when the intrinsic 329 viscosity of the CAID material is lower, transient piles tend to collapse and spread over 330 the CMB following interaction with downwellings that push the dense component into high 331 structures. As the intrinsic viscosity contrast,  $\Delta \eta_C$  is increased, events leading to compres-332 sion, and to higher and less wide piles (e.g., due to the impact of neighbouring downwellings), 333 leave longer-lived signatures in stiffer piles. An inverse trend is also observed between the 334 buoyancy number and the height of CAID material piles so that cases with a buoyancy 335 number of 0.75 typically feature greater height piles than cases with a buoyancy number of 336 1.0. A potential impact on the dynamics responsible for the formation of the plates results 337 from a decrease in the relative viscosity of the CAID material (e.g., when it is hot and not 338 intrinsically higher in viscosity) or an increase in buoyancy number. Both factors lead to 339 an increase in CMB blanketing by the dense component. Increased coverage of the CMB 340 can lead to a cooler mantle in comparison to an isochemical case. For example, a blanket-341 ing layer, or discrete piles, can inhibit heat flow from the core. As a result, mean global 342 viscosity is affected by both the buoyancy number and the intrinsic viscosity of the CAID 343 material and, in turn, a resulting difference in plate behaviour can determine the number of 344 downwellings able to form and therefore whether CAID material disperses into one or more 345 piles. In summary, the findings from our 2D calculations indicate that a higher intrinsic 346 viscosity for the CAID material promotes degree-1 mantle flow, especially for cases with 347 reduced buoyancy ratio. 348



Figure 2. Temperature (top) and composition (bottom) field snapshots featuring a range of buoyancy numbers (columns) and CAID material intrinsic viscosities (rows). The temperature scale is the same as in Fig. 1. Red and blue in the composition fields correspond to values of 1.0 and 0.0, respectively.

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### 3.4 Thermal state time-dependence and CAID material distribution

Figure 3 presents snapshots of the thermal and compositional fields from Models 350 2DB0.75D100 and 2DB0.75D10, as well as basal and surface heat flux time series for the 351 three cases from Fig. 2 featuring a buoyancy number of 0.75. In general, mean heat flux is 352 minimally influenced by the intrinsic viscosity of the CAID material, however, variation be-353 tween maximum and minimum surface heat flux values is reduced when there is no intrinsic 354 contrast in viscosity between the different compositions (most likely because the predom-355 inantly degree-one-flow cases are more impacted by the opening and closing of a smaller 356 number of plate boundaries). Red and blue vertical lines are annotated on the heat flux 357 time series, indicating the timing of the snapshots shown. Both times are selected for their 358 relation to a spike in surface heat flux, which occurs following the transition from a sys-359 tem with a single downwelling to periods featuring the development of a new surface weak 360 zone (resulting in the formation of second downwellings that supersede the existing down-361 wellings which subsequently dissipate). Pre-existing long lasting downwellings appear in the 362 southern and northern hemispheres for cases 2DB0.75D100 and 2DB0.75D10, respectively, 363 while young downwellings are seen to form in the northern and southern hemispheres in the 364 same cases. For case 2DB0.75D100 it is observed that mean surface heat flux increases by 365 approximately  $21 \text{ mW/m}^2$  following the initiation of a downwelling in the northern hemi-366 sphere. The basal heat flux is observed to have a similar response to the development of new 367 downwellings. However, throughout the period modelled, the basal heat flux varies over a 368 narrower range of values with a slightly delayed response. 369

Sudden variations in heat flux associated with the development and loss of surface 370 downwelling regions indicate the transient nature of these calculations. A similar frequency 371 in the rate of heat flux variation is observed for all three cases presented in Figure 3 with 372 each case experiencing at least one rapid increase in surface heat flux per Gyr, indicating 373 the formation of a new zone of convergence forms in the calculations at intervals of 1 Gyr or 374 less. Generally, changes in the amplitude of the heat flux time variations also coincide with 375 changes in the nature of the CAID material's distribution due to the feedback between the 376 surface motion and intrinsically dense component. 377

Figure 4 is similar to Figure 3, but illustrates the evolution of cases where  $\Delta \eta_c = 100$ . For reference, Model 2DB0.75D100 appears (in red) again. Solid vertical lines are used to indicate the time corresponding to each snapshot at the left. The snapshot of Model



Figure 3. (Thermal and compositional field snapshots from Models 2DB0.75D100 (left) and 2DB0.75D10 (right) and the corresponding CMB (dashed) and surface (solid) mean heat flux time series. Heat flux is shown in dimensional units of  $mW/m^2$  by using the values from Table 1, while dimensional time is provided on the top x-axis and non-dimensional (diffusion) time is given on the bottom axis. The times corresponding to each snapshot are indicated on the heat flux plots by a vertical line of the same colour as the associated heat flux curves.

2DB0.75D100 features a high surface heat flux and two downwellings, while the snapshot 381 from Model 2DB1.0D100 corresponds to a period of low heat flux and the existence of only 382 a single region of subduction. In comparison to Model 2DB0.75D100, Model 2DB1.0D100 383 exhibits significantly lower minimum surface heat flux values during its evolution. These 384 are associated with the intermittent cessation of surface convergence, and therefore down-385 wellings, and the replacement of a continually mobile surface with an episodic regime of 386 convection. Correspondingly, this case features the highest average internal temperatures 387 of all of the 2D calculations presented. Thus we find that in a 2D system, a combined high 388 buoyancy number and intrinsic viscosity contrast can lead to a disruption of the large scale 389 flow owing to intermittent stagnation of the surface. 390

Figure 5 shows the thermal and compositional field evolution for Models 2DB0.75D100 and 2DB1.0D100. The sequence on the left depicts two distinct piles of anomalously dense material occupying opposite hemispheres throughout the illustrated period. Additionally, the surface of this system features two zones of localized convergence that result in the consistent preservation of widely separated regions of downwelling. The focused subducting material impinges upon the CAID material near the core mantle boundary, forming voids in which no CAID material is present above the CMB. Additionally, as exhibited by the



Figure 4. (Thermal and compositional field snapshots for Models 2DB0.75D100 (left) and 2DB1.0D100 (right) and the corresponding CMB (dashed) and surface (solid) mean heat flux time series. Heat flux is plotted in dimensional units of  $mW/m^2$  while dimensional time is provided on the top x-axis and non-dimensional (diffusion) time is shown on the bottom axis. The times corresponding to each snapshot are indicated by a solid vertical line of the same colour as the associated heat flux curve. Dashed vertical lines bound the time ranges presented in Figure 5.

- northern hemisphere evolution between 0.95 and 1.58 Gyr, downwelling lithosphere can act
  to further shape CAID material into narrower piles with steeper sides. Moreover, the height
  of the piles in the two hemispheres can differ by roughly a factor of two.
- Model 2DB1.0D100 displays a greater transience in the CAID material distribution 401 over a slightly shorter period; initially two diametrically opposed piles are present, which 402 coalesce into a single pile before breaking apart again. Unlike Model 2DB0.75D100, the sur-403 face of Model 2DB1.0D100, features only a single region of focused convergence throughout 404 the illustrated period. Accordingly, the system is less efficiently cooled by subduction and 405 is persistently hotter. At time 0 Gyr, downwelling material originating near "two o'clock" 406 sinks to the core mantle boundary driving the CAID material to move laterally about the 407 CMB. At time 0.52 Gyr, the downwelling material has spread over the CMB forcing the 408 CAID material into a single pile covering most of the CMB in the opposite hemisphere. At 409 0.78 Gyr, downwelling at two o'clock ceases and a new region of downwelling forms above 410 the centre of the CAID province. By 1.04 Gyr, the downwelling has generated a new void 411 in the CAID material coverage of the CMB and has re-established a two pile distribution. 412
- These two cases illustrate the impact of plate convergence on the formation of diametrically opposed provinces. More than one persistent downwelling is required for long term



**Figure 5.** A series of thermal and compositional field snapshots for Models 2DB0.75D100 (left) and 2DB1.0D100 (right) displaying the evolution of each case over approximately 1.5 Gyr. An age is indicated next to each set of annuli images indicating the time that has passed since the top-most panel. The times corresponding to the first and last snapshot are indicated by dashed vertical lines in Figure 4. The temperature scale is the same as in Fig. 1.

maintenance of two diametrically opposed provinces. Subduction initiated over a void in
CAID material coverage of the CMB will enforce the coalescing of material into a single
pile, while subduction initiated over a province will often divide the province into two piles.
If, in the latter case, the subduction is robust and long lasting the piles will once again
coalesce into a single province in the opposite hemisphere. Of final note, feedback between
the CAID material and plate convergence zones can result in global temperature changes
that are conducive to the intermittent cessation of surface mobility.

422

## 3.5 Three-dimensional convection calculations

Although we expect some of the behaviour observed in two-dimensional calculations 423 to be maintained in three-dimensional systems (e.g., the impact of the intrinsic viscosity 424 contrast of the two component system as well as the influence of the buoyancy number 425 on province height and total core coverage), the limited degrees of freedom in the two-426 dimensional system can result in dynamics that will not be reproduced in a full spherical 427 shell; suggesting the potential for some departures from the 2D behaviour. For example, 428 the CAID material piles formed in 2D systems break apart and disperse over the CMB 429 in a similar way to the modelling of supercontinent breakup and dispersal at the surface 430 of the mantle (Gurnis, 1988). However, limitations caused by restricting the migration of 431 distinct components, like continental lithosphere (Zhong & Gurnis, 1991) or CAID material 432 provinces (Langemeyer et al. 2020), to motion on a great circle can force cycles that are 433 unlikely to be realized in three-dimensions, or eliminate realistic alternatives for evolution 434 that require three dimensions. For example, 2D systems can only model supercontinent 435 cycles that replicate end-member paradigms for ocean opening and closure, rather than the 436 spectrum of possibilities that actually exist (Murphy & Nance, 2004, Rolf et al., 2012). 437 Moreover, in two dimensions, changes in the direction of the migration of a dense province 438 requires reversals, as with changes in plate motion (e.g., Lowman et al., 2001). In the case of 439 plate motion this restriction can introduce episodicity (Koglin et al., 2005), including brief 440 periods of stagnation, and therefore an affect on global temperatures. 441

A 3D model will allow for different options in the location, relative orientation and distribution of downwellings originating along bands of surface convergence. In the remainder of this study, we focus on how the feedback between downwellings and CAID material affects the formation of CAID provinces within a 3D system. Additionally, we analyze the impact of the CAID material component on the evolution of localized regions of deformation at the surface. Specifically, we investigate whether a two component deep mantle affects
the mobility of plates and whether the contrasting structure of convergent and divergent
surface features is persistent; as observed in the isochemical calculation (Langemeyer et al.,
2021).

In addition to the uniform  $(2 \times 10^7; 110 \text{ MPa})$  yield stress calculations that allow for 451 a direct comparison with the two dimensional model results, we investigate the impact of a 452 reduction in the surface yield stress on the interior thermal structure and the distribution of 453 CAID material. In this case, the surface yield stress has been weakened by a factor of two 454 but increases linearly until reaching a non-dimensional depth of 0.02 (60 km), below which 455 the yield stress is again set at a constant valued  $2 \times 10^7$ . This alternative model is conducive 456 to generating more convergent bands that result in downwellings (although, for isochemical 457 models, it is much less effective in producing a dichotomy in the structure of divergent and 458 convergent boundaries; marked by the appearance of transform faults in the former case). 459 The choice of investigating cases with a weaker surface is prompted by an understanding 460 that the CAID material is driven into piles by its interaction with downwellings, and that 461 adjusting a primary factor affecting the formation of downwellings may have a profound 462 effect on recovering a system with a pair of distinct provinces and a plate tectonic-like 463 surface. 464

#### 465

#### 3.6 Initial condition for the 3D calculations

Figure 6 presents snapshots of the initial conditions used for the 3D calculations. 466 Figure 6a shows viscosity and divergence field snapshots for the initial condition used to 467 start all 3D calculations featuring a uniform yield stress. In addition, the interior thermal 468 structure is displayed utilizing hot and cold isosurfaces corresponding to focussed upwelling 469 and downwelling material, respectively, as well as the corresponding temperature field power 470 spectrum (horizontal) as a function of non-dimensional height (vertical) above the CMB. 471 Similarly, Figure 6b shows the initial condition utilized for all depth-dependent yield stress 472 calculations described. The initial conditions were generated from calculations in which a 473 CAID component is absent. In the uniform yield stress case, the surface features just three 474 plate-like regions at the time shown, however, for the parameters selected, half-a-dozen 475 plates often evolve. Moreover, the parameters are identical to those chosen in the earlier 2D 476 computations and have demonstrated compatibility with the generation of distinct CAID 477 provinces in that geometry. The surface zones of convergence and divergence are distinct 478

in their structure with the former appearing as smooth continuous (arcuate) bands and the 479 latter appearing as a series of spreading centres (analogous to ridges) punctuated by offsets 480 (analogous to transform faults). The depth-dependent yield stress case exhibits an initial 481 condition featuring more distinct plate-like regions but less well defined divergent boundaries 482 (and no transform-like offsets). The surface shows a number of zones of focused deformation 483 and power across a band of harmonics (peaking at degree three). The cases presented in 484 the remainder of this study are initiated from these fields with a uniform thickness layer 485 of CAID material (accounting for 3.0% of the mantle volume) enveloping the CMB, unless 486 noted otherwise. 487

488

## 3.7 CAID material distribution in three-dimensional calculations

Figure 7 presents snapshots from nine calculations incorporating intrinsically dense 489 material with different buoyancy numbers and viscosity contrast owing to composition. 490 These cases all feature a uniform non-dimensional yield-stress of  $2 \times 10^7$ . In addition to 491 the viscosity field just below the surface, a hot interior isosurface and the CAID material 492 distribution are shown. The rendering of the surface viscosity field utilizes the same colour 493 definitions as the images presented in Figure 6, while the red and blue isosurfaces show a 494 thermal cut-off of non-dimensional temperature 0.82 and the distribution of CAID material, 495 respectively. For the same cases, images from temporally corresponding but diametrically 496 opposed viewing angles are presented in Supplementary Figure 1. For a number of cases, 497 following the introduction and evolution of the CAID material, similar divergent and conver-498 gent surface features to those exhibited in the isochemical initial condition are maintained. 499 In addition, the length-scale of these plate boundaries is maintained in many cases, with 500 long bands of deformation persisting for a mantle transit time or longer, such as in Models 501 3DB1.0D10 and 3DB0.85D100 which exhibit focussed weak zone bands subtending 180°. 502 Some snapshots, such as for Model 3DB1.0D1, display a surface with a greater number 503 of weak zones (as revealed by the near surface power spectrum) resulting in an increased 504 number of isolated surface regions analogous to distinct plates. However, in all cases, far 505 fewer plate-like regions are found than is currently observed on Earth. 506

A variety of CAID material distributions are shown in Figure 7, however, despite frequent sampling, none of the cases examined with this yield stress model were found to produce a persisting pair of CAID material provinces, as would be analogous to the structure of the LLSVPs observed at the base of Earth's mantle. Supplementary Figure 2



Figure 6. The initial conditions used for the initiation of uniform yield stress  $(2 \times 10^7; 110 \text{ MPa})$  3D calculations (a) and cases with a depth-dependent yield stress (surface =  $1 \times 10^7$ , interior =  $2 \times 10^7$ ) (b). Near surface viscosity and non-dimensional divergence as well as internal thermal structure and its power spectra (as a function of height above the CMB) are presented for each case. The thermal isosurfaces correspond to non-dimensional temperatures of 0.82 (red) and 0.42 (blue). The left and right columns show diametrically opposed views. Cold isosurfaces are clipped at a non-dimensional depth of 0.05 to reveal the thermal interior structure. All 3D model calculations are carried out in a spherical geometry utilizing a yin-yang grid with a resolution of  $96 \times (768 \times 256) \times 2$  and 930 million tracers.

presents Mollweide projections of the compositional field 145 km above the CMB in nine 511 plots corresponding to the snapshots shown in Fig. 7. The most common distribution of 512 CAID material observed is that of a single large pile, typically extending over an area of 513 at least one hemisphere. Generally, large voids are carved out of the dense layer by robust 514 downwellings sinking to the core mantle boundary. Some smaller piles of CAID material are 515 seen in Model 3DB1.0D100 of Figure 7 and Model 3DB0.85D10 of Supplementary Figure 1. 516 Only a small amount of the total CAID component is included in these isolated piles and 517 typically they tend not to be completely detached, but rather are connected to the larger 518 piles by tendrils of the CAID component reaching across the CMB. As was found in the 519 study of the 2D cases, the height and steepness of the piles appears to be greatest when the 520 intrinsic viscosity of the dense component is large relative to the ambient mantle. Those 521 cases where  $\Delta \eta_C$  equals 100 feature the greatest altitude and steepest sided piles. In accord, 522 these cases can also exhibit less core coverage by the CAID component. A low buoyancy 523 number CAID component is less resistant to being forced aside by cold downwelling material. 524 Consequently downwellings can push a lower buoyancy ratio dense component laterally as 525 the reduced density of the piles means they are more readily deformable as well as able to 526 rise to higher altitudes. Furthermore, CAID material with an increased  $\Delta \eta_C$  will respond 527 more slowly to the opportunity to spread around the core mantle boundary during periods 528 when the pile experiences diminished lateral forcing. 529

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#### 3.7.1 Temperature field power spectra

For each case in Fig. 7 a plot of the thermal power spectra as a function of height 531 above the CMB is shown in Supplementary Figure 3. The power spectra indicate the 532 dominant degrees in the upper thermal boundary layer as well as the distribution of the 533 CAID material in the deep mantle. Long wavelength peaks in the power spectra near the 534 surface of the systems are typical, with the greatest power usually occurring at degree one or 535 two, corresponding to the number and spacing of bands of focussed surface deformation. In 536 addition to the strong degree one or two surface power observed, a subset of cases including 537 Models 3DB1.0D1 and 3DB0.85D100 display some power in higher degrees. In particular, 538 these cases feature a greater number of bands of lithospheric weakness traversing shorter 539 distances across the surface. The power focused in the lowest degrees in the mantle, just 540 above the CMB, results from the influence of CAID material distribution and is generally 541 much stronger than focusing observed at the surface. Due to the relatively low buoyancy of 542



**Figure 7.** Snapshots from the nine uniform yield stress 3D cases featured in this study. The buoyancy number and intrinsic viscosity contrast for the CAID material and ambient mantle are indicated at the left and bottom of the figure, respectively. For each case, the viscosity field is shown at a depth of 0.005*d* juxtaposed with a (to scale) image of the mantle interior illustrating CAID material distribution (in blue) and thermal plumes (transparent red, non-dimensional temperature of 0.82). (The viewing angle of the viscosity field and model interior are the same.) The temperature power spectra corresponding to each snapshot is presented in Supplementary Fig. 3.

the CAID material, a large amount of heat is trapped in the dense provinces so that thermal 543 power spectra indicate the nature of the intrinsically dense material's distribution. As with 544 the power spectra at the surface, predominantly degree-one to -two power is observed, 545 indicating that the CAID material is typically grouped into a single large pile but that a 546 capacity for distribution into two piles exists. Cases featuring a buoyancy number of 1.0 547 display power in harmonics as high as degree 3 (and 4), most likely because those cases 548 exhibit a higher occurrence of shorter, localized, near-surface, deformation zones that (2D 549 results indicated) are capable of promoting small isolated piles (e.g., Model 3DB1.0D100) 550 or simply more discontinuity of the CAID layer. We note that the locations associated with 551 surface weakening are not clearly imprinted on the underlying CMB by an absence of CAID 552 material. This suggests that the migration of lithospheric weak zones may be at least as fast 553 as the rate of arrival of sinking material at the CMB. However, as in the two-dimensional 554 systems analyzed, we find that the arrival of downwellings at the CMB pushes aside CAID 555 material so that its distribution is largely influenced by plate convergence. The results of 556 the three-dimensional cases indicate that an apparent influence of the feedback between the 557 plate boundary distribution and CAID material placement is the similar focus in low degree 558 powers. Model 3DB1.0D10 is one of the two cases shown that features its strongest power 559 at the surface in the degree two signature. It is examined in detail in section 3.7.3. 560

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#### 3.7.2 Transience in the heat flux

Figure 8 displays heat flux time series for the three cases appearing in Figure 7 featuring 562 a buoyancy number of 0.75. We find no clear impact on the trend of the CMB heat flux values 563 or their temporal variation for the range of intrinsic compositionally originating viscosity 564 contrasts examined. As in the 2D calculations employing the same parameters (Figure 3), 565 the surface heat flux is highly time-dependent, however, it shows less variation in the 3D 566 calculations (e.g., when comparing the ratios of maximum to minimum value). In the two-567 dimensional cases, roughly 100% increases in surface heat flux are possible while the largest 568 swing in heat flux in the 3D cases is closer to 50%. Consistent with the 2D results of Figure 569 3 we observe that spikes in heat flux are associated with the initiation of new downwellings. 570 The 3D downwellings are structurally more complicated than the 2D downwellings but a 571 greater degree of freedom is present in fully spherical environments. Thus, smoother and less 572 dramatic variations in amplitude occur between periods of low heat flux and high heat flux 573 because surface velocities do not need to slow when plates change direction. For example, 574



Figure 8. Surface and basal heat flux time series for the three 3D cases with uniform yield stress featuring a buoyancy number of 0.75. Green, blue and red correspond to cases where  $\Delta \eta_C$  equals 1, 10 and 100, respectively. The time series illustrate surface and basal heat flux values using solid and dashed lines, respectively.

in a 2D model, if one convergent boundary closes while another emerges, plate directions 575 can reverse and velocity briefly drops to zero. However, in 3D, changes in plate direction do 576 not require a reduction in the global surface velocity and the initiation of new subduction 577 zones is less impactful on surface heat flux. A notable difference between the 2D and 3D 578 calculations is that the variation in heat flux was reduced when  $\Delta \eta_C = 1$  in 2D cases, which 579 was attributed to the prevailing degree-2 flow in this case, versus a degree-1 trend in the 580 other cases. In the 3D cases, we do not observe such a trend in heat flux or a clear contrast 581 in the power spectra harmonics, we attribute this to the added degree of freedom of the 582 3D systems that removes the discretized contrast between degree-1 and degree-2 flow. One 583 similarity between the two-dimensional and three-dimensional models is that increases in 584 surface heat flux typically correspond to an increase in heat flux at the CMB. 585

Figure 9 presents heat flux time series for the three cases shown in Figure 7 featuring  $\Delta \eta_C = 100 \text{ (n.b., Model 3DB0.75D100 (red) appears in both figures). In contrast to the three$ cases in Figure 8 with a common buoyancy number, these heat flux profiles show a trend.



Figure 9. Surface and basal heat flux time series for the three 3D cases with uniform yield stress, featuring CAID material with an intrinsic viscosity that is 100 times greater than the ambient mantle. Red, cyan and black correspond to cases where B = 0.75, 0.85 and 1.0, respectively. The time series illustrate surface and basal heat flux values using solid and dashed lines, respectively.

The heat flux diminishes as the buoyancy ratio is increased (this can be seen most clearly in 589 the basal heat flux times series). Furthermore, for a corresponding CAID material viscosity 590 the buoyancy number 0.75 cases are hotter in 3D calculations. The transience of surface 591 and basal heat flux is again observed but the transition from periods of low heat flux to 592 high heat flux occurs over longer periods and the range of minimum and maximum heat flux 593 values is narrower than in the analogous 2D cases. The basal heat flux trend agrees with 594 the findings of the 2D calculations which demonstrated that an increased buoyancy number 595 can result in greater insulation of the CMB. 596

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### 3.7.3 Evolution of the plate boundaries and CAID material distribution

We now examine the detailed time-dependence of one of the cases from Figure 7. The time-averaged power spectrum for the temperature field of Model 3DB0.75D10 showed a peak in lower mantle power at degree 2. A period of 1 Gyr of evolution (ending at the time

shown in Figure 7) is analyzed here in order to determine whether this spectral peak ever 601 corresponds to two distinct provinces. 602

Figure 10 displays six sequential snapshots of the near surface viscosity field as well 603 as isosurfaces that reveal plumes (red, non-dimensional temperature of 0.82) and CAID 604 material distribution (blue) for Model 3DB0.75D10. Each row shows an instant in time as 605 viewed from diametrically opposed positions. Additional viewing angles are presented in 606 Supplementary Figure 4. The viscosity field shows the evolution of features such as narrow 607 weak bands (corresponding to convergence and divergence) that bound the low strain-rate 608 plate-like regions. In addition, at times 200 Myr and 400 Myr the viscosity fields display 609 the formation, evolution and dissolution of transform-like offsets along spreading bound-610 aries. The feedback between surface features and the distribution of the CAID material is 611 illustrated in the column marked  $0^{\circ}$  in Fig. 10 , from times 600 Myr to 1 Gyr. The snapshot 612 at time 600 Myr features CAID material that forms a great province extending from the 613 northern to southern pole. At time 800 Myr the previously discontinuous convergent bands 614 in the left and right hemispheres (roughly coincident with the equatorial region in the figure) 615 have merged, forming a triple junction with a spreading boundary located in the southern 616 hemisphere. The merging of the convergent boundaries has lead to the development of a 617 sheet-like downwelling that plunges into the deep mantle and impacts the CAID material 618 below, pushing aside the dense material. Accordingly, the north-to-south pole extending 619 province becomes split into a north and south fragment. In general, large voids are present 620 in the CAID material below convergent surface features. Conversely, spreading boundaries 621 incorporating transform offsets are most typically found over regions of the CMB covered by 622 CAID material. This characteristic mimics the behaviour observed in the two-dimensional 623 cases. 624

625 626

We note that in this calculation, the movement and repositioning of the CAID material's periphery on the CMB occurs on the same time scale as the motion of the plate boundaries. Accordingly, plumes anchored at the peripheries of the CAID provinces migrate at 627 similar rates. Some plumes form on top of the CAID material piles, below divergent surface 628 features, but they lack the vigour needed to penetrate into the upper mantle. 629

In Supplementary Figure 5 we present Mollweide projections of the compositional field 630 145 km above the CMB for each of the times corresponding to Fig. 10. Given the full  $360^{\circ}$ 631 view of the CAID material shown in Supplementary Fig. 5 a brief period of two province 632

formation is revealed at 0 Myr. However, unlike Earth's LLSVPs, the separation of the provinces is relatively small. Moreover, it does not persist. This period marks the only time we observe the formation of two provinces. The distribution of the CAID material in this epoch apparently produced the degree-2 signature in the time averaged power spectrum of the model's thermal field.

Given the evidence that downwellings drive the formation of regions on the CMB that 638 are void of CAID material, we explored the dependence of the distribution of the CAID 639 material on downwellings by reducing the surface yield stress to allow for a greater number 640 of convergent bands in the model lithosphere. Model 3DB0.75D100weak is similar to Model 641 3DB0.75D100 except that it employs the weaker yield stress model described in section 3.6 642 and initializes by placing a CAID layer in the thermal field shown in Fig. 6b. The yield 643 stress increases with depth over the top 2% of the mantle from a non-dimensional surface 644 value of  $1 \times 10^7$  to a uniform yield stress of  $2 \times 10^7$  at all lower depths. 645

Figure 11 presents a series of snapshots for Model 3DB0.75D100weak. The viscosity 646 field snapshots exhibit the increased number of convergent and divergent surface bands 647 resulting from the weakening of surface yield stress, leading to the development of a greater 648 number of downwellings and individual plates. (However, with the weakened surface the 649 calculation no longer exhibits the transform-like offsets punctuating divergent features.) The 650 increased number of smaller scale downwellings leads to a greater number of voids within 651 the layer of CAID material. For example, multiple voids are observed in the column marked 652  $0^{\circ}$  at time 540 Myr in Fig. 11; column B at time 900 Myr of Supplementary Figure 6; 653 and column D times 360 to 720 Myr (also Supplementary Figure 6); varying in size and 654 number. Accordingly, the CAID material tends to form a greater number of narrow tendril-655 like features joining the piles on the CMB, as exhibited in the columns marked  $0^{\circ}$  of Fig. 656 11 and  $90^{\circ}$  (B) in Supplementary Figure 6. 657

<sup>658</sup> Supplementary Figure 7 shows the compositional field 145 km above the CMB at the <sup>659</sup> times presented in Figure 11 and illustrates the growth and movement of voids in the dense <sup>660</sup> layer rather than coalescing of the dense material into piles. The formation of numerous <sup>661</sup> connecting branches between larger nodes occasionally allows for the isolation of a fraction <sup>662</sup> of the CAID material into small, short-lived piles. This is exhibited in the 0° column at <sup>663</sup> times 540 to 900 Myr, where a small pile is loosely connected to the greater mass of CAID <sup>664</sup> material by narrow tendrils, briefly isolated (e.g., at 720 Myr in Supplementary Figure 7)



Figure 10. Snapshots of the near surface viscosity field and CAID material distribution at six different times (rows) throughout the evolution of Model 3DB0.75D10. Diametrically opposed viewing angles are presented for each time, with the angle of rotation relative to a vertical axis through the centre of the sphere in the left-most column indicated at the top of the second column. Additional viewing angles are presented in Supplementary Figure 6.

and then rejoined to the larger pile through another narrow tendril. The weakening of the surface yield stress thus leads to the formation of a greater number of small scale features at the surface (including downwellings) and a CAID distribution on the CMB that might be described as 'fragments connected to a large province incorporating voids'. However, aggregation into two similar volume provinces is not obtained during the more than 1 Gyr modelled.

Figure 12 shows thermal power spectra as a function of height above the CMB for the model presented in Figure 11. Although the distribution of the CAID material during this period appears unchanged from a qualitative perspective, the thermal power spectra indicate a field dominated by degree-2 above the CMB has transitioned to a field with a degree-1 signature, in addition to lesser power distributed as high as degree-6. Given their hot signatures we infer that periods dominated by degree-2 CAID material distribution occur, but detection of such a period is not an indicator of a pair of detached provinces.

To explore the possibility that the critical issue inhibiting the formation of two dis-678 tinct provinces in our calculations is the specification of an excessive volume of the CAID 679 material, we examined a final case incorporating a reduction in the volume of the intrin-680 sically dense component. Model 3DB0.75D100weak&reduced employs identical parameters 681 and initial condition to Model 3DB0.75D100weak but the CAID component incorporated in 682 the calculation comprises only 2% of the mantle volume. Figure 13 shows the evolution of 683 Model 3DB0.75D100weak&reduced by presenting the divergence field and temperature field 684 power spectra as a function of height above the CMB. The corresponding evolution of the 685 near surface viscosity field and thermal power spectra is presented in Supplementary Figure 686 9. The corresponding evolution of the dense layer is shown in Supplementary Figure 10. As 687 in the other calculations presented, at time 0.0 Myr the mean temperature of the model has 688 equilibrated following the incorporation of the CAID layer into the initial condition thermal 689 field (Fig. 6b) and subsequent forward modelling. Although the reduction in the volume of 690 the CAID component does not result in a pair of distinct provinces during the evolution of 691 this case, the introduction of the denser material does have a global impact on temperature 692 that results in the formation of a greater number of distinct plates and triple junctions than 693 in either the isochemical initial condition models or the previously described case (Model 694 3DB0.75D100weak) featuring a higher volume of CAID material. Moreover, the divergent 695 boundaries exhibit multiple examples of transform-like offsets (e.g., the boundary extending 696 'north-south' in the column marked 180°). The influence of a CAID mantle component on 697



Figure 11. Snapshots of the near surface viscosity field and CAID material distribution at six different times (rows) throughout the evolution of Model 3DB0.75D100weak. Diametrically opposed viewing angles are shown for each time with the angle of rotation relative to the left-most column indicated at the top of the columns. Supplementary Figure 6 presents additional viewing angles of the viscosity field and CAID material distribution at the same times.



Figure 12. Thermal field power spectra as a function of height above the CMB for the case presented in the previous figure. The timing of the spectra presented corresponds to the first and final frames shown above.

the formation of plates is illustrated by the impact of plates and dense provinces on the temperature field of the systems examined.

Figure 14a depicts temperature profiles taken from the initial condition models in 700 Fig. 6 (red and cyan curves) as well as time-averaged profiles from the cases presented in 701 Figs. 10, 11 and 13 (magenta, green and blue, respectively) and shows the impact on global 702 temperature of both a weakened lithospheric yield stress and the presence of a hot CAID 703 component sitting on the CMB; specifically the insulation of the mantle from core heat flow 704 that emplacement of this component engenders. The influence of a lower lithospheric yield 705 stress is revealed by comparing the red and cyan curves, which show the substantial cooling 706 resulting from a greater number of downwelling sheets that form with a lowered yield stress. 707 With the addition of the CAID material, temperature increases in the lowest 15-20% of the 708 mantle relative to the isochemical cases. The increased temperature extends to a smaller 709 height above the CMB in the case where the volume of the intrinsically dense material is 710 reduced (blue curve). In all cases featuring a CAID component, the mantle above the deep 711 layer incorporating the CAID component is cooler than in the corresponding isochemical 712 case because the denser material sitting on the core reduces heat flow into the mantle. The 713 degree of mid-mantle cooling is clearly determined by the volume of the CAID material. This 714 is illustrated by comparing the green and blue curves: the lower volume of CAID material in 715 Model 3DB0.75D100weak&reduced (blue) results in a warmer mantle in that case, relative 716 to that of Model 3DB0.75D100weak (green), above the depths that incorporate the CAID 717 material. (At the same time, the blue curve is cooler than the magenta because the model 718 producing the latter has a weaker surface and allows for a longer network of interior-cooling 719 (convergent) plate boundaries.) However, the blue curve (2% CAID material) is hotter than 720 the cyan (no CAID material) in the upper mantle and the cyan curve is just mildly warmer 721 than the green (3% CAID material). This departure from the other systematic trends is a 722 manifestation of what is effectively a regime change in the lithospheric character. The cyan 723 curve (the initial condition model with a weaker lithospheric yield stress) corresponds to a 724 case with a mobile surface but less distinct plates and boundaries than in the uniform yield 725 stress cases. Adding the 2% CAID component to the mantle has affected global flow so that 726 a cooler mid-mantle and hotter upper mantle evolves. The result is conducive to producing 727 more clearly defined plates isolated by tightly focussed boundaries. 728

729

Figure 14b shows the viscosity profiles corresponding to the temperature profiles in 14a, emphasizing that the heat trapped in the CAID material counteracts the high intrinsic



**Figure 13.** Snapshots of the near surface non-dimensional velocity divergence field and CAID material distribution at six different times (rows) throughout the evolution of Model 3DB0.75D100weak&reduced. Diametrically opposed viewing angles are shown for each time with the angle of rotation relative to the left most column indicated at the top of each column. Additional viewing angles are shown in Supplementary Figure 8.
viscosity of the dense components to such a degree that the isochemical cases exhibit the 731 highest mean viscosity in the region between the deepest five and fifteen percent of the 732 mantle. The viscosity profiles also show the impact of robust deep penetrating slabs. For 733 example, although hotter at mid-mantle than Model 3DB0.75D100weak, the viscosity profile 734 from the initial condition case with a depth-dependent yield stress shows a higher averaged 735 viscosity. The high mean viscosity is explained by the incorporation of numerous very high 736 viscosity downwellings into the averaging. The exponential law for the viscosity has a large 737 impact on averaging where slabs are present while slabs have a relatively smaller impact on 738 mean temperature at a given height. This effect also produces small scale gradient variation 739 in the viscosity profiles relative to the smoother temperature profiles, particularly in the 740 isochemical (initial condition) cases. 741

Previous authors (e.g., Stein et al., 2004; Stein & Hansen, 2008; Höink et al., 2012; 742 Lenardic et al., 2019) have described the critical role of mid-mantle temperatures and vis-743 cosity increase with depth on the generation and sustained mobility of plates. The findings 744 presented here illustrate that the presence of a compositionally anomalous and intrinsically 745 dense mantle component can impact the mid-mantle temperature profile in a way that in-746 fluences the global viscosity profile and therefore plate formation and mobility. Finally, 747 lowered lithospheric yield stress and a greater volume of CAID material cool the mantle 748 overall. However, as described above, the intrinsically dense mantle component becomes 749 particularly hot. The combined affects of its temperature and intrinsic density result in a 750 much more marginal increase in the density of the CAID component than is implied by the 751 buoyancy numbers. We discuss this further below. 752

#### 4 Discussion 753

754

Although the origin and physical characteristics of the LLSVPs are contentious, with the exception of secondary details there is broad agreement on the physical bounds and 755 seismic properties of the regions of the mantle that define the locations of the provinces 756 (e.g., Cottaar & Lekic, 2016). Specifically, whatever the cause of the seismic signature, the 757 vast majority of the volume of the mantle satisfying classification as LLSVP is divided into 758 a pair of detached features. The distribution of a chemically distinct volume of the mantle 759 into two distinct features blanketing approximately 30 percent of the CMB while rising 760 over 1000 km above the CMB (Garnero et al., 2016) provides key constraints on efforts 761 to determine the physical properties of the compositionally anomalous material assumed 762



Figure 14. Temporally averaged profiles of the latitudinally and longitudinally averaged temperature (a) and viscosity (b) as a function of height above the core mantle boundary in five of the 3D geometry cases featured in this study. The red curve corresponds to the isochemical initial condition model with a uniform yield stress; the cyan curve corresponds to the isochemical case with the depth-dependent yield stress; the magenta, green and blue curves correspond to Models 3DB0.75D10, 3DB0.75D100weak and 3DB0.75D100weak&reduced, respectively.

responsible for the observation of LLSVPs. Obtaining two detached provinces comprised 763 of such material is not a default distribution of the inclusion of such a component in a 764 3D spherical shell. In contrast, recovering a pair of large provinces is not as an elusive 765 outcome in two-dimensional models, including the spherical annuli modelled in the first part 766 of this study. We suggest that the challenge of identifying the physical properties of the 767 CAID material that yields LLSVP-type distributions in 3D shells is somewhat analogous 768 to identifying the properties of a fluid mantle that yield sheet-like downwellings. (Two-769 dimensional calculations with mobile surfaces always produce this desired behaviour, but 770 obtaining slab-like downwelling morphology in 3D spheres is limited to a set of systems with 771 very specific material parameters, initial conditions and shell thicknesses.) 772

A deficiency of the 3D models that is mostly likely explained by the absence of dis-773 crete CAID provinces and a core largely free of coverage by the dense component, is the 774 scarcity of vigorous plumes, capable of transiting the entire depth of the mantle. Given 775 the inferred association of plume generated igneous provinces with chemically originating 776 LLSVPs (Torsvik et al., 2006; Burke et al., 2008; Li & Zhong, 2017; Heyn et al., 2020), 777 the relatively small number of plumes is counter to the expectation of observing PGZs. 778 However, this result is consistent with the observed broad coverage of the CMB by CAID 779 material. Plume generation zones have been inferred to form at the boundaries of relatively 780 small footprint provinces, where thermal gradients can generate plumes. Adjacent to the 781 provinces are broad expanses of the CMB where high heat flow can be drawn into the man-782 tle and advected towards province boundaries. In the 3D cases presented here, the CAID 783 material forms expansive punctured layers with voids that may be too small to draw enough 784 heat from the CMB to allow the formation of robust plumes. In contrast, Langemeyer et 785 al. (2021) found examples of several vigorous plumes transiting the mantle in an isochemi-786 cal model employing the same parameter values as the 110 MPa uniform yield stress cases 787 presented here. The generally reduced heat flux (and therefore support for plumes) at the 788 CMB, found when CAID material is added to the calculations, is illustrated in Figs. 8 789 and 9. The contribution to surface heat flow from the core, indicated by the time series in 790 these figures, is in the 10-15% range. This is at the lowest end of widely accepted estimates 791 of CMB heat flow (e.g., Lay et al., 2008). Figure 14 shows that a strong sub-adiabatic 792 temperature profile exists in several models due to slabs pooling in the deep mantle. A sub-793 adiabatic temperature profile will also decrease the temperature anomaly that characterizes 794 rising plumes. 795

Overall, our findings do agree with previous studies. By assuming that the origin of 796 the LLSVPs is explained by a chemically distinct lower mantle component, we conclude 797 that the buoyancy ratio of this material (relative to the ambient mantle) as well as an 798 inherent viscosity contrast between the intrinsically dense component and remaining mantle 799 material, both impact the distribution, durability and mobility of the CAID component. 800 For example, when all other system parameters are held constant, increasing the intrinsic 801 viscosity of the denser mantle component tends to result in degree-1 flow, in contrast to 802 the degree-2 structure more readily obtained in the isochemical or chemically enriched cases 803 where  $\Delta \eta_C = 1$ . 804

We have excluded the influence of compressibility in our calculations but do not expect this omission to impact the overall dynamics of the systems described given the scale height of the mantle (of order  $10^7$ m.). Nevertheless, compressibility is responsible for decreasing thermal expansivity in the lower mantle. Accordingly, in estimating the total density anomalies occurring in the CAID provinces in these calculations, due to both chemical and thermal affects, an adjustment of the mean thermal expansion coefficient value given in Table 1 is necessary.

For the range of buoyancy numbers considered (0.75, 0.85 and 1.0), the dimensional 812 increase in the density of the enriched mantle component is  $138.75 \text{ kg/m}^3$ ,  $157.25 \text{ kg/m}^3$ 813 and  $185 \text{ kg/m}^3$ , respectively, for a comparison of surface temperature materials (equating 814 with density increases of 3.75%, 4.25% and 5%). However, these contrasts must be adjusted 815 when temperature contrast between the CAID and ambient mantle material is considered. 816 Moreover, in the lowermost mantle, the thermal expansion coefficient may be up to 50%817 lower than its upper mantle value. As illustrated in Fig. 2, the dense provinces are typically 818 1000-1250 K (0.4 to  $0.5\Delta T$ ) hotter than the ambient mantle, so that thermal influence, com-819 bined with a reduction in the thermal expansion coefficient, reduces their density contrast 820 when compared to the ambient mantle (assuming a thermal expansion coefficient of  $1 \times 10^{-5}$ 821  $K^{-1}$  and an ambient mantle nondimensional temperature of 0.5). Accordingly, the CAID 822 material provinces modelled are thus approximately 0.625% to 1.5% more dense than the 823 adjacent mantle at the same depth. Actual density anomalies associated with the LLSVPs 824 remain an issue of debate (e.g., McNamara, 2019), but may be encompassed within this 825 range. However, in these models, the primary factor that determines the choice of the in-826 trinsic density contrast between the enriched and ambient mantle components is ultimately 827 the requirement of the durability of the denser volume of the two-component system. For 828

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models in which the denser component is not replenished, such as in this study, the specification of a buoyancy number below 0.7 results in entrainment and mixing of the dense layer given vigorous convection persisting over time periods of a few billion years. Our calculations (and the implied minimum and maximum density anomaly they yield between the ambient mantle and chemically distinct regions) result in a density anomaly estimate that is consistent with that inferred from seismic observations (Trampert et al. 2004).

Our study imposed the requirement that plate-like surface motion should be exhibited 835 for calculations producing LLSVP-type piles on the CMB, if model outcome is to be con-836 sidered applicable to understanding the feedback between surface dynamics and the Earth's 837 deep interior. This requirement is especially important because plate-like surface behaviour 838 produces strong focussed downwellings in the mantle (slabs) and these features have the 839 greatest impact on the distribution and mobility of the CAID material (e.g., McNamara 840 & Zhong, 2005; Zhang et al., 2010). However, the simultaneous modelling of dynamically 841 evolving plates and thermochemical piles increases the number of variables in the system 842 so that the cases presented here comprise coverage of a small fraction of the possible cases 843 that may be relevant to Earth's evolution. Despite this, some specific behaviour appears 844 to be general. A small number of thermochemical piles are not readily obtained in the 3D 845 calculations. Instead, downwelling sheets penetrate CAID material layers to produce a dis-846 tribution better described as a layer punctuated by multiple holes. Decreasing the volume 847 of the CAID material tends to reduce the mean thickness of the layer featuring the holes 848 rather than prompting the separation of the dense material into piles. Moreover, decreasing 849 the volume of the dense component is contrary to non-consensus estimates of the volume 850 of the LLSVPs which are as great as eight percent of the mantle's volume (Cottaar & Le-851 kic, 2016). As described by numerous other authors, decreasing the buoyancy number of 852 the denser component can allow for the formation of higher topography, reduced 'footprint' 853 piles, but this occurs at the expense of pile durability. In the models we present, which as-854 sume a primordial, non-renewing, CAID component, a lower buoyancy number is conducive 855 to mixing and dissipation of the dense component (e.g., Trim et al., 2020). Possible future 856 avenues for investigation that may reconcile the existence of two thermochemical piles in 857 a spherical shell exhibiting plate tectonics may require the modelling of a renewing source 858 lower buoyancy number material for the CAID component than was consider in this study. 859 However, this may be problematic (Brandenburg & van Keken, 2007; Li & McNamara, 2013) 860 rather than offering a solution. Nakagawa et al. (2010) and Nakagawa & Tackley (2011) 861

862 863 employed sophisticated three-dimensional spherical models in which the dense material was produced by melting but also did not obtain two piles in the systems studied.

In contrast, studies that have imposed plate velocity on 3D spherical shells have read-864 ily obtained two LLSVP-like features for anomalously dense mantle components similar in 865 volume, relative density and viscosity to those investigated here. The difference in our find-866 ings and those of investigations that imposed recent plate motion history (e.g., McNamara 867 & Zhong, 2005; Zhang et al., 2010) may result from a lack of feedback in the former studies 868 but could also stem from the neglect of continents in the work presented here. The breakup 869 of a supercontinent might impact the number of piles obtained in the deep mantle. For 870 example, dispersing continents (or the process of supercontinent breakup) may play a role 871 in organizing subduction in a way that results in a dominant degree-2 convection pattern 872 that simultaneously promotes two thermochemical provinces (e.g., Li & Zhong, 2009; Li & 873 Zhong, 2017). However, exploring the feedback between a CAID component, continents and 874 the modelling of dynamic oceanic plates remains a computational challenge in 3D systems 875 with Earth-like convective vigour so that studies will be strongly limited by the number of 876 variables that can be investigated. 877

Despite the difficulty of obtaining two LLSVP-like provinces from the addition of a 878 CAID component to a 3D model, two-dimensional components not only readily produce 879 two distinct piles but can also emulate some of the other seismically inferred morphology. 880 For example, at time 1.58 Gyr in Fig. 5, the calculation featuring a buoyancy number of 881 0.75 exhibits one province that rises approximately 1000 km above the CMB while the other 882 province is just half that height. Together the provinces cover about 30% of the CMB. These 883 figures mimic the approximate dimensions of the LLSVPs determined by seismic studies, 884 including the greater volume and height of the African anomaly (e.g., Cottaar & Lekic, 885 2016). In general, the time-dependence of the CAID material features in the 2D calculations 886 take on a variety of shapes that can mimic cross-sections of LLSVP images. Specifically, 887 the intrinsically dense provinces are more likely to take on heights in excess of 1000 km 888 or more above the CMB when the buoyancy number is in the 0.75 - 0.85 range and the 889 intrinsic viscosity contrast between the enriched and surrounding material is much greater 890 than one. However, we note that we model a uniform distribution of internal heat sources. 891 For higher buoyancy number, enrichment of the CAID material with a greater degree of 892 internal heating (e.g., Li et al., 2019) could produce higher topography features than those 893 found in our study. Nevertheless, the findings presented from this study are cautionary, in 894

that they show that conclusions regarding the physical properties of the LLSVPs, inferred from the morphology of dense components in 2D thermochemical models do not always reproduce LLSVP-like features in 3D systems.

A similar issue exists with regard to modelling plates in the presence (or absence) of a 898 two-component lower mantle. The modelling of plates affects system heat flow at both the 899 upper and lower boundaries. Dramatically different system behaviour is therefore possible 900 in models featuring the modelling of plates, when the heating conditions are identical. For 901 example, the presence of a CAID component partially blanketing the CMB reduces heat 902 flow into the mantle and therefore results in a cooler interior. The result of a cooler mantle 903 is analogous to reducing the internal heating rate of the mantle, which has been shown in 904 multiple studies employing plate modelling methods (e.g., Stein et al., 2014) to promote 905 surface mobility. Similarly, the presence of a CAID component in the lower mantle can 906 affect the formation of plate boundaries because of the impact of reduced mantle temper-907 ature on the tractions that break the model lithosphere. In addition, the two-dimensional 908 calculations in our study showed not only that slabs could impact, deform and split CAID 909 material provinces but that the provinces would instil convective patterns that would result 910 in repeated failure of the lithosphere in the same narrow region. Thus, the modelling of 911 plates and the inclusion of a CAID mantle component results in a feedback that appears to 912 affect both CAID material distribution and plate boundary locations. A potential disrup-913 tion to the establishment of such feedback might be provided by the inclusion of continents 914 in these models or the change in the limited degree of freedom for plate motion that ac-915 companies three-dimensionality. Accordingly, we conclude that the physical properties of 916 a CAID mantle component that will promote the formation of a pair of distinct provinces 917 may require the modelling of continents covering about 30% of the mantle's surface. 918

# <sup>919</sup> 5 Conclusion

Tectonic plate motion has been a corollary of terrestrial mantle convection (e.g., Bercovici, 2003; Coltice et al., 2017; 2019; Crameri et al., 2019) for more than a billion years (Dhuime et al., 2015). Consequently, investigating the evolution of the current structure of the deep interior with global-scale mantle convection calculations requires modelling a system yielding the primary aspects of plate tectonics: the existence of focussed sheetlike downwellings (slabs), persistent piece-wise uniform surface motion, and the presence of evolving plate boundaries. Previous work has shown that mantle convection models featur-

ing methods for reproducing or generating plate-like surface velocity fields (e.g., Monnereau 927 & Quéré, 2001; Lowman et al., 2001; Lenardic et al., 2019) exhibit internal temperature 928 structure (and therefore viscosity) that differs from systems with other surface behaviour. 929 Principally, this effect is produced by the influence that plates have on mantle heat loss. 930 The presence of chemically dense provinces lying on the core mantle boundary have been 931 shown (Langemeyer et al., 2020) to inhibit heat flow into the mantle and therefore also 932 affect mantle temperatures (and viscosity). Here we show that for modest volumes (2-3.5%)933 of the mantle) the impact of incorporating a compositionally anomalous and intrinsically 934 dense component in mantle convection calculations can change temperature profiles so that 935 plate-like surface behaviour is obtained for different parameter values from those required 936 for isochemical models. 937

Presenting results from eleven vigorously convecting 3D calculations, we also show 938 that obtaining a pair of compositionally distinct provinces with LLSVP-like coverage of the 939 CMB is elusive in systems featuring dynamically evolving plate-like surfaces. Not only does 940 the presence of a CAID component in the mantle affect the surface velocity field character, 941 but a pair of enduring provinces did not evolve in any of the cases that we considered. In 942 contrast, two-dimensional systems exhibit a pair of diametrically opposed provinces for a 943 range of model parameters. We highlight the significance of flow direction in explaining 944 this discrepancy. The CAID material in a 2D model can only flow in two lateral directions. 945 Accordingly, slab impact above a dense province inevitably divides the existing feature into 946 two detached components and drives the resulting features in opposing directions. The 947 additional degrees of freedom in a 3D calculation allow for flow of the CAID material to 948 move so that the intrinsically denser material can become perforated by the arrival of a 949 slab but not necessarily divided. Moreover, a mass of CAID material can be split from a 950 perimeter location inwards to a radial hinge-point, around which the material will effectively 951 rotate in a nearly horizontal plane while never separating into two detached masses. 952

The cases we present here are far from exhaustive in terms of the values considered for CAID material density contrast or viscosity contrast. Similarly, the values specified in our calculations for the key parameters governing plate formation represent a small subset from just one possible rheological description of mantle flow. However, the findings illustrate a few fundamental issues that are likely to prevail in further studies. Namely, the obtaining of LLSVP-type features from thermochemical mantle components is not an inevitable system outcome, particularly when a simultaneous requirement for a plate-like surface is also imposed; the inclusion of a CAID component in a model can be either conducive to
encouraging the generation of a plate-like surface velocity field or detrimental to producing
plates; and intrinsically dense mantle components may remain rooted in the deep mantle
while trapping enough heat within so that their relative contrast in density (and viscosity)
with the surrounding mantle is much less than implied by the comparative properties at a
common temperature.

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# 973 Code Availability

The computer code, STAGYY, used for all calculations described herein can be obtained upon reasonable request from P.J. Tackley.

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1	Supplementary Figures:
2	Contrasts in two- and three-dimensional system
3	behaviour in the modelling of compositionally
4	originating LLSVPs and a mantle featuring dynamically
5	obtained plates
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Figure 1. Snapshots of the nine uniform yield stress 3D cases featured in the study. The buoyancy number and intrinsic viscosity contrast for the CAID material and ambient mantle are indicated at the left and bottom of the figure, respectively. For each case, the viscosity field is shown at a depth of 0.005*d* juxtaposed with a (to scale) image of the mantle interior illustrating CAID material distribution (in blue) and thermal plumes (transparent red, non-dimensional temperature of 0.82). The viewing angle of the viscosity field and model interior pairs are the same and they are diametrically opposed to the viewing angle of the corresponding cases in Fig. 7.



Figure 2. Mollweide projections of the composition field, C, on a surface 0.05d above the CMB. The panels correspond to the nine snapshots presented in Fig. 7 (and Supplementary Fig. 1). Buoyancy ratio is fixed in each row and the viscosity contrast between the intrinsically dense and ambient mantle (when both are at the CMB temperature) is fixed in each column. Blue corresponds to regions of the CMB blanketed by CAID material.



**Figure 3.** Power in the thermal fields presented in Fig. 7 (and Supplementary Fig. 1), as a function of spherical harmonic and non-dimensional height above the CMB.



**Figure 4.** Snapshots of the near surface non-dimensional viscosity field and CAID material distribution at six different times (rows) throughout the evolution of Model 3DB0.75D10. The angle of rotation relative to a vertical axis through the centre of the sphere in the left-most column is indicated at the top of each column. The viewing angles used in Fig. 10 are presented for each time in the columns labelled A and C.



Figure 5. Mollweide projections of the composition field, C, on a surface 0.05d above the CMB from Model 3DB0.75D10. The panels correspond to the six snapshots presented in Fig. 10 (and Supplementary Fig. 4). Blue corresponds to regions of the CMB blanketed by CAID material.



**Figure 6.** Snapshots of the near surface non-dimensional viscosity field and CAID material distribution at six different times (rows) throughout the evolution of Model 3DB0.75D100weak. The angle of rotation relative to a vertical axis through the centre of the sphere in the left-most column is indicated at the top of each column. The viewing angles used in Fig. 11 are presented for each time in the columns labelled A and C.



Figure 7. Mollweide projections of the composition field, C, on a surface 0.05d above the CMB from Model 3DB0.75D100weak. The panels correspond to the six snapshots presented in Fig. 11 (and Supplementary Fig. 6). Blue corresponds to regions of the CMB blanketed by CAID material.



**Figure 8.** Snapshots of the near surface non-dimensional velocity divergence field and CAID material distribution at six different times (rows) throughout the evolution of Model 3DB0.75D100weak&reduced. The angle of rotation relative to a vertical axis through the centre of the sphere in the left-most column is indicated at the top of each column. The viewing angles used in Fig. 13 are presented for each time in the columns labelled 0° and 180°.



Figure 9. Snapshots of the near surface non-dimensional viscosity field and thermal power spectra at six different times (rows) throughout the evolution of Model 3DB0.75D100weak&reduced. The snapshots shown correspond to the velocity divergence field snapshots shown in Supplementary Fig. 8. The viscosity field is shown at a depth of 0.005*d*. Four viewing angles are shown for each time, with the angle of rotation relative to the left most column indicated at the top of the figure. The power spectra of the temperature field at the corresponding time is shown in the right column as a function of non-dimensional height above the CMB and spherical harmonic degree.



**Figure 10.** Mollweide projections of the composition field, *C*, on a surface 0.05*d* above the CMB from Model 3DB0.75D100weak&reduced. The panels correspond to the six snapshots presented in Fig. 13 (and Supplementary Fig. 8). Blue corresponds to regions of the CMB blanketed by CAID material.