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How to assess similarities and differences between mantle circulation models and Earth using disparate independent observations

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Mantle circulation in the Earth acts to remove heat from its interior and is thus a critical driver of our planet's internal and surface evolution. Numerical mantle circulation models (MCMs) driven by plate motion history allow us to model relevant physical and chemical processes and help answer questions related to mantle properties and circulation. Predictions from MCMs can be tested using a variety of observations. Here, we illustrate how the combination of many disparate observations leads to constraints on mantle circulation across space and time. We present this approach by first describing the set-up of the example test MCM, including the parameterization of melting, and the methodology used to obtain elastic Earth models. We subsequently describe different constraints, that either provide information about present-day mantle (e.g. seismic velocity structure and surface deflection) or its temporal evolution (e.g. geomagnetic reversal frequency, geochemical isotope ratios and temperature of upper mantle sampled by lavas). We illustrate the information that each observation provides by applying it to a single MCM. In future work, we shall apply these observational constraints to a large number of MCMs, which will allow us to address questions related to Earth-like mantle circulation.

1. Introduction

Our planet's evolution and present-day state are ultimately driven by convection in its deep interior. This convection is partially controlled by subducting slabs at destructive plate margins, and partially by thermal upwellings initiated at thermal boundary layers. While the locations of cool subducting slabs and hot plumes are reasonably well constrained close to the surface of the Earth, their positions, morphologies and time-dependent behaviour in the lower mantle remain poorly constrained.

Models of global mantle convection can now include phase transitions, coupling between composition and density, compositional tracking, decompression melting and surface motions driven by plate history models. The predictions of these simulations over recent Earth history to present-day can be tested with disparate observations that can help to constrain mantle flow. Such work has been done over the last two decades with increasing sophistication, primarily focusing on seismic and surface topography observations for constraints (e.g. [1–11]).

In this paper, we demonstrate how suites of observations—with different sensitivities to the spatio-temporal evolution of the mantle—can be used to test predictions from MCMs (see figure 1). The specific constraints used here have been selected with the goal of providing a broad coverage of this four-dimensional space, something that will ultimately give the best chance of constraining MCMs. These observations come from a wide range of disciplines, including seismology, surface deflections, geomagnetism, petrology and geochemistry. We first present the simulation method. We then, in turn, discuss the geophysical or geological context of each observation, together with the relevant predictions from an actual MCM (case m_cc_066_u) for that observation. We note that this MCM is a not very Earth-like sample model and that our constraints are not exhaustive; many other observations could be used, e.g. hiatus maps, body-wave travel times [13] and lithospheric stress field (see other contributions to this special issue). What is novel here is both some of the individual constraints and the breadth of constraints applied simultaneously.

2. Mantle circulation modelling

Our mantle circulation models (MCMs) use models of recent plate motion history as surface-velocity boundary conditions. This gives plate tectonic-like surface velocities in locations consistent with geological history on Earth [1–6,14,15]. Predictions from the MCMs enable geographical comparisons. These includes comparisons with observations that are independent of horizontal surface motions. Our long-term goal is to use such comparisons to constrain the properties of the mantle, for example, the viscosity of the mantle and the density of recycled oceanic crust. A better understanding of its viscosity, which controls the rate of flow of the mantle, would for example allow one to address the question of how quickly slabs sink in the mantle [16]. Knowledge of the density of recycled metamorphosed oceanic crust, which controls how/if it segregates from the bulk flow, would allow one to address the question: to what extent does recycled oceanic crust contribute to the large low seismic velocity provinces (LLSVP) of the lowermost mantle [17]?

We simulate mantle dynamics by solving the conservation of mass, momentum, energy and composition equations in global three-dimensional spherical geometry, following [18–22]. Details of our MCM modelling are presented in the supplemental material (electronic supplementary material, table S1), with a brief summary presented here. The simulation presents a compressible mantle, assuming an anelastic approximation using a Murnaghan equation of state (see Bunge *et al.* for details [20], with a depth-varying coefficient of thermal expansion and reference density). The lateral surface velocities arise from the plate motion history of Müller *et al.* [23], applied from 1 Ga to present-day in 1 Myr steps, scaled to the natural velocity of the model, avoiding forced convection. We also ensure zero surface radial velocities, while the core-mantle boundary (CMB) velocity boundary condition is free-slip. The surface and CMB are isothermal, with the surface kept at 300 K, while notably, the temperature of the core evolves self-consistently over time using the coupled model of Davies [24]. The resulting CMB heat flux evolution is presented in electronic supplementary material, fig. S2.

The model is thermochemical and tracks bulk composition using a single parameter, C, which varies from $C = 0$ (harzburgite-like), through $C = 0.2$ (lherzolite-like) to $C = 1$ (basalt-like), advected on particles. For simplicity, we use the terms harzburgite, lherzolite and basalt to represent these compositions, even in regions of the mantle where the mineralogy is changed and these terms do not strictly apply. The basalt is assumed to be more dense than the average mantle in the lower mantle (buoyancy number = 0.66; see electronic supplementary material). It is less dense between 660 and 720 km to replicate the delayed phase transformations in the basalt component, which some have argued can produce a basalt barrier [25]. The model includes the dynamic influence of phase boundaries at 410 and 660 km depth (see electronic supplementary material). We also implement self-consistent melting following Van Heck *et al.* [22] when the source temperature exceeds its solidus. This produces a surface layer enriched with basalt, which is recycled into the mantle in regions of plate convergence. The melting also considers partitioning of tracked elements according to their partition coefficient and the degree of melting. The tracked elements include the heat-producing radiogenic isotopes and their daughters (Th, U, K, Pb, He, Ar).

The rheology of the mantle is assumed to have a temperature-dependent Newtonian viscosity. The radial reference profile includes a lower viscosity in the upper mantle (4×10^{21} Pa s), a higher viscosity in the lithosphere (×100) and lower mantle (×30), which decreases to a low viscosity (×1) as we descend towards the hot CMB (electronic supplementary material, fig. S3). The simulation presented here uses the benchmarked [21], parallel [19] code TERRA [14,18,20,22,26–28], with an average lateral resolution at mid-mantle depth of approximately 45 km, with similar radial spacing.

3. Producing isotropic seismic structure from MCMs

The outputs of the thermochemical MCMs (temperature and composition at a given pressure/computational node) serve as inputs for extracting rock physical properties from tables produced from phase equilibrium calculations, outlined below.

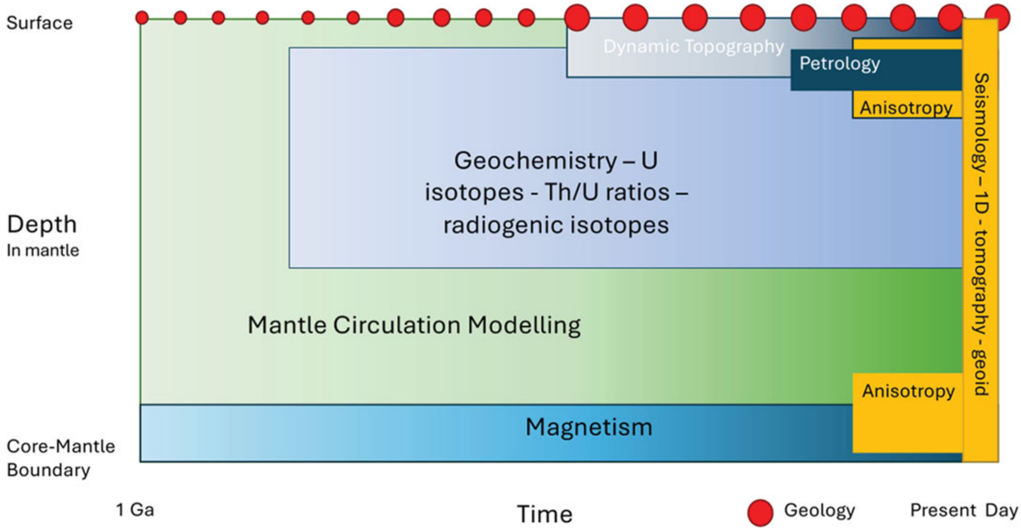

Figure 1. Schematic showing where in space (illustrated schematically over mantle depth) and time we might expect different constraints and models to constrain global mantle circulation. The size of geology symbols reflects the number of observations while the shading hints at likely sensitivity of constraint. Different aspects of seismology will constrain different depths, e.g. fundamental mode surface wave data primarily constrain the shallow mantle, while Stoneley modes add constraints about the lower mantle. Some aspects like dynamic topography and geoid can have specific sensitivity kernels that this figure cannot represent. Inspired by Gerya [12].

In general, the compositional value C on the particles and the fine mesh ($0.0 < C \leq 1.0$) correspond to enrichment relative to harzburgite. However, because only one C value is tracked, an intermediate value could correspond to a single lithology or a mechanical mixture of multiple lithologies [29]. To determine seismic velocities from P, T and C, we must therefore first make an assumption about how C maps to the local lithology. In our approach, we assume that our models are composed of mechanical mixtures of three discrete bulk compositions. If $0.0 \leq C < 0.2$, the rock is assumed to be a mixture of harzburgite and lherzolite with proportions varying linearly with the C value, otherwise, it is assumed to be a linear mixture of lherzolite and basalt for $0.2 \leq C \leq 1$.

Throughout this paper, we assume that harzburgite, lherzolite and basalt have constant bulk compositions (electronic supplementary material, table S3), assuming the compositions reported by Baker & Beckett [30] (harzburgite), Walter [31] (lherzolite) and White & Klein [32] (basalt). The physical properties of lherzolite, harzburgite and basalt are calculated using a Gibbs free energy minimization, as implemented in Perple_X [33] using the equation of state of Stixrude and Lithgow-Bertelloni [34–36]. We use the mineral dataset provided in [36] and available at github.com/stixrude/HeFESTo_parameters_010121. This provides thermodynamic and elastic properties for each of the bulk compositions, stored as three separate P-T property tables. As the mineral dataset lacks a covariance matrix, we cannot propagate parameter value uncertainties into uncertainties for the calculated physical properties. However, as a first-order approximation, we estimate an average uncertainty in V_s of approximately 0.4% for harzburgite and lherzolite and approximately 1% for basalt (see electronic supplementary material, S2). We expect the uncertainties in V_p to be of a similar magnitude. The effective isotropic seismic velocities for each bulk composition are corrected for anelastic effects using model Q7g [37,38], which produces a good agreement with published studies on attenuation [39]. Final effective densities and seismic velocities throughout the domain are calculated by harmonic averaging of the lherzolite, harzburgite and basalt material, weighted by the mass fractions f_i^M of each bulk composition (see electronic supplementary material).

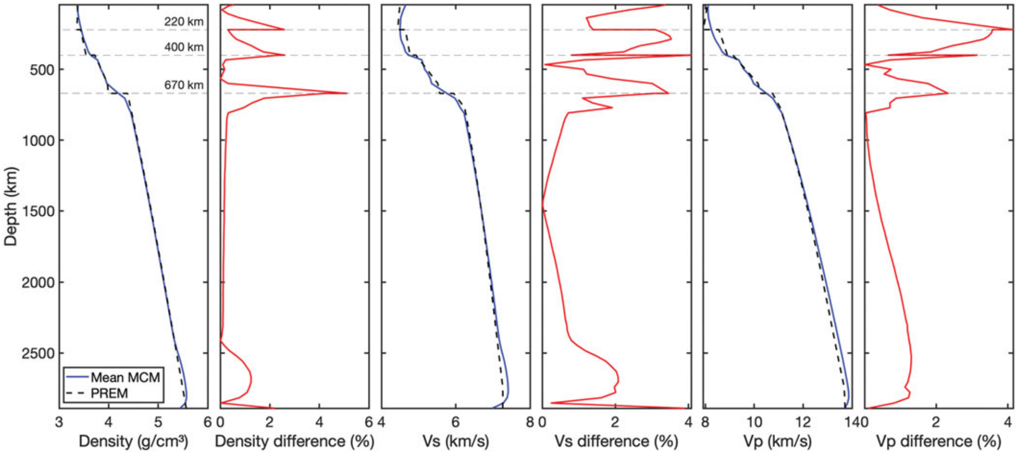

Figure 2. Comparison of the one-dimensional average density, V_s and V_p profiles of the MCM (blue lines) compared with PREM (black dashed lines). Red lines show the absolute difference in per cent between the models. Dashed horizontal lines at 220, 400 and 670 km depth represent the major seismic discontinuities in PREM.

4. Testing models with seismic observations

Seismology provides primarily a snapshot of the present state of the Earth's mantle (figure 1), with a wide range of possible observations that can be used to test predictions of an MCM. Here, we present a subset only, to give an example of what is possible. Many of these seismic constraints have already been considered in other studies [13,40], but typically not all together.

(a) Whole mantle

(i) One-dimensional isotropic

The one-dimensional radially averaged seismic structure of the Earth is an obvious choice for a metric with which to test MCMs [41]. This structure primarily depends on the bulk composition of the mantle as well as the average temperature (geotherm), properties which are usually tracked in MCMs. The conversion to seismic velocities is achieved by thermodynamic modelsets of mineral phases, which are increasingly well-constrained by inversions of high-quality experimental data [34–36,42]. The synthetic one-dimensional structure can be readily compared with high-quality models created by inversion of seismic data [41,43]. A comparison of the radially averaged one-dimensional profile extracted from our example MCM with PREM [41] is shown in figure 2. The radially averaged structure of our example MCM matches PREM well below approximately 800 km depth (within 1–2%), but in the bottom approximately 400 km in the mantle, the deviations from PREM increase (figure 2). This is possibly due to the compositional gradient in the MCM, where the recycled oceanic crust preferentially collects at the base of the mantle. Such unexpected deviations can be used to identify and in future potentially reject poorly performing MCMs.

Figure 2 also highlights some of the caveats that come from a naive comparison between one-dimensional radially averaged velocity structure and velocity structure obtained from seismic data. The first is that the synthetic structure exhibits smooth increases in velocity approximately 410 km and 660 km depth. These smooth increases are a consequence of averaging sharp transitions that take place at different depths due to the temperature dependence of the olivine-wadsleyite and ringwoodite-breakdown reactions. The discrete jumps in the PREM and AK135 models arise because those models are built on seismic data that are sensitive to the magnitude and depths of jumps in seismic velocity, rather than one-dimensional radial structure [44]. At depths shallower than 400 km, discrepancies are due both to the lack of continental lithosphere in

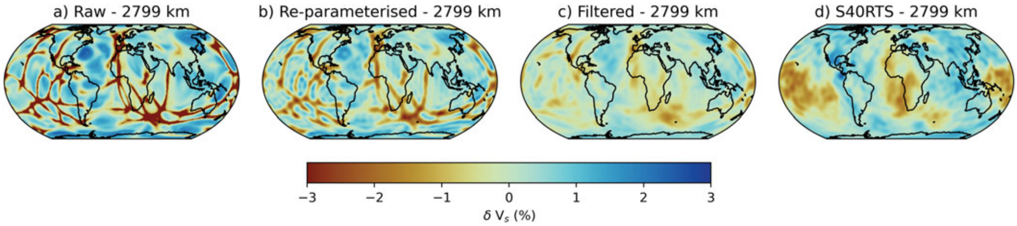

Figure 3. Example of tomographic filtering of an MCM. (a) High-resolution δV_s at 2799 km depth from MCM simulation. (b) Re-parameterized δV_s up to spherical harmonic degree 40. (c) Filtered δV_s using the resolution operator for tomography model S40RTS. (d) Seismic tomography model S40RTS.

the MCM, and a lack of mineralogical justification for a 220 km discontinuity proposed in PREM. Note that, the 220 km discontinuity does not exist in AK135 [43]. Further details are provided in electronic supplementary material, S3.1.1.

(ii) Three-dimensional long-wavelength tomography

Seismic tomography provides a snapshot of the present-day state of the mantle, with numerous models developed since the 1980s. While these typically differ in detail, especially for V_p, the long-wavelength (e.g. spherical harmonic degree $\lesssim 12$) isotropic V_s structure has been consistently imaged by different studies (for a review, see [45]). The strength of V_s anomalies depends primarily on the temperature variations in the mantle, which in turn depends on many factors such as mantle viscosity structure, CMB temperature and internal heating rates. The observed pattern and amplitude of V_s anomalies can thus be used to test several parameters of the MCM.

Due to uneven data coverage and imposed regularization, tomographic models of the Earth have limited and spatially variable resolution. To compare the high-resolution, predicted seismic structure of our MCM with published tomographic models, we must therefore adjust the predicted seismic structure using the resolution operator from existing tomography models. Alternative approaches for tomographic filtering include the generalized inverse projection method [46]. While some studies allow for separate filtering of V_p and V_s [47], tomographic studies do not consistently image the V_p structure. Here, we use tomography model S40RTS [48], which has often been used in comparisons with geodynamic simulations (e.g. [4]) and for which a tomographic filter is available. The MCM is first re-parameterized in the same parameterization as the tomographic model [40], e.g. spherical harmonic coefficients up to degree 40 across 21 radial splines [49], before the resolution operator is applied (figure 3).

After filtering, the predicted seismic velocity structure can be compared quantitatively to the tomography model itself. Such comparisons could focus on particular regions or depths, but the exact location of seismic velocity anomalies may differ, e.g. differences in reference frames of plate reconstructions [50]. It is, therefore, more useful to compute the correlation at each spherical harmonic degree, which indicates whether the structures are of similar wavelengths and at similar locations for relevant depths. We note though that strong correlation does not require similar amplitude. An example of this is given in figure 4, where we also show the total correlation for each radial layer up to spherical harmonic degree 8 and 20. A strong positive correlation between S40RTS and the predicted structure of the MCM is found throughout the lower mantle up to spherical harmonic degree 4–5, while the correlation in the upper mantle is higher on average. We also condense the correlation spectra into a single number by computing the weighted mean correlation, accounting for the change in area with depth. For the simulation presented here, the volume-weighted mean correlation with S40RTS up to degree 40 is 0.35. This compares favourably to the critical value at a 99% significance level ($r_{\mathrm{crit}} = 0.014$). Such weighted mean correlation values can be used as a metric to rank a range of simulations to a given tomography model, to assess their relative success in reproducing global seismic structure. This analysis can be

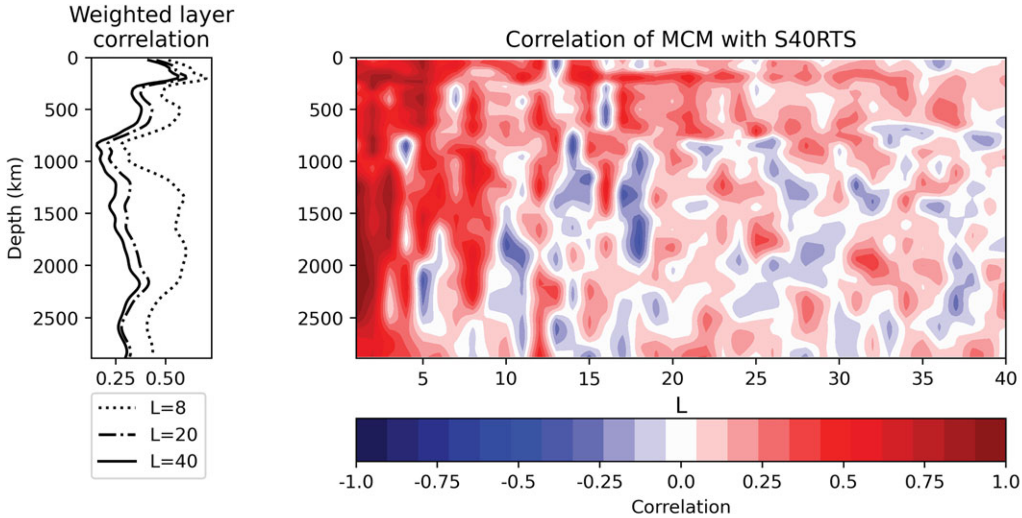

Figure 4. Comparison of the MCM with seismic tomography. Left panel: total correlation between the filtered, predicted V_s structure of the MCM and seismic tomography model S40RTS, up to spherical harmonic degree $l_{\max} = 8$, $l_{\max} = 20$ and $l_{\max} = 40$. Right panel: correlation per degree up to degree 40 as a function of depth.

performed for the entire mantle, or separately for different depth regions. It can also be extended to V_p, e.g. using the SP12RTS filter [47]. This would also make it possible to investigate ratios and correlations of seismic velocities, which inform about phase transitions in the mantle.

(iii) Normal mode splitting

Earth's normal modes are standing seismic waves that arise after large earthquakes. Their resonance frequencies are affected by Earth's rotation, ellipticity and internal structure, including three-dimensional variations in seismic velocities and, crucially, density [51]. Observations of lateral variations in resonance frequencies (so-called splitting function maps) thus provide a way to assess several aspects of the MCMs, albeit only on long wavelengths, e.g. [52]. We illustrate the constraints that normal modes provide by comparing synthetic splitting function maps predicted by the MCM with observations from [53,54] for two groups of modes with specific sensitivity: 10 fundamental modes that are sensitive to the upper mantle and 10 Stoneley modes that are increasingly sensitive to the deepest mantle (see electronic supplementary material). For upper mantle modes (black dots in figure 5), the MCM prediction matches the observation reasonably well, both in amplitude and pattern (quantified by the correlation and amplitude ratio). However, for lower mantle modes (e.g. figure 5a–b), the splitting function maps feature similar high-frequency anomalies (typically interpreted as cold mantle, downwellings), but the low-frequency regions (hot mantle, upwellings) are typically shifted with respect to the observations, resulting in a lower correlation. Although we only analyse 10 modes in each group, this difference is more apparent for lower mantle (blue dots) than for upper mantle (black dots) modes (see electronic supplementary material, fig. S2). This suggests that in addition to assessing the overall mantle structure, normal mode splitting is also a good test for the plate motion history model used in geodynamic simulations [55].

(b) Upper mantle

The upper mantle is studied more widely and better constrained seismically, and many different observations exist that might be used to constrain MCMs. Here, we consider one-dimensional

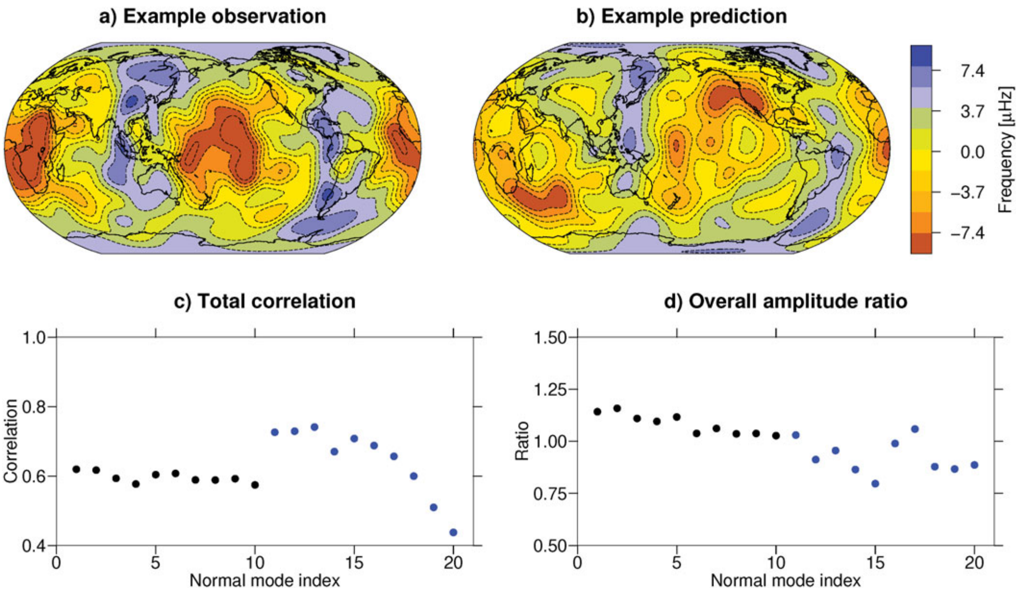

Figure 5. Quantitative assessment of the MCM using normal mode splitting. (a) The observed splitting function map for lower mantle spheroidal mode ${}_1S_{10}$ with the MCM prediction for the same mode shown in (b). (c,d) The total spectral correlation and spectral amplitude ratio for 10 upper mantle modes (black circles) and 10 lower mantle modes (blue circles). These are always computed up to the maximum spherical harmonic degree of the observed splitting function map.

radial anisotropy, phase velocity maps and subtractive optimally localised average (SOLA) surface wave tomography to illustrate the use of both indirect data and tomography.

(i) One-dimensional radial anisotropy

Seismic velocity structure as discussed above provides a snapshot of the final state of the model. However, in principle, two MCM runs could have very different histories of flow but converge to the same thermal and compositional structure at the present-day, resulting in the same isotropic structure. Seismic anisotropy in the mantle is believed to be controlled by the history of deformation (e.g. [56]), so may be an effective discriminant between MCMs with different pasts (e.g. [57]). However, the prediction of seismic anisotropy from MCMs is computationally challenging compared with the prediction of the isotropic signal, and there are additional assumptions behind both the calculation of model values, and results obtained from observation. Seismic anisotropy has been observed (at least regionally) across the whole depth range of the mantle (e.g. [56]), but here we restrict ourselves to the upper 400 km of the mantle. This has the advantage of having the best established mineralogical behaviour, and a well-studied radial anisotropy (both in one and three dimensions). The simplest comparison is the average variation with depth of (shear-wave) radial anisotropy. This captures the general character of the shallow flow field without focusing on regional detail, and is readily compared with a one-dimensional (e.g. PREM [41]) or averaged three-dimensional (e.g. [58–60]) model. To calculate the radial anisotropy associated with an MCM, we have assumed upper mantle anisotropy is dominated by the formation of crystallographic preferred orientation in olivine and extended the approach described in [61–67]. Further details are given in the electronic supplementary material, S3.2.1. This approach results in a model of the elastic structure of the upper mantle described by 21 independent elastic constants at each location. For comparison with observation, we reduce this to radial anisotropy and focus on the S-wave anisotropic parameter ξ $(=(V_{\mathrm{SH}}/V_{\mathrm{SV}})^2)$.

The global radial variation of ξ for our example MCM is shown in figure 6. This is evaluated at each 50 km depth interval by averaging 162 evenly laterally distributed points. The comparison

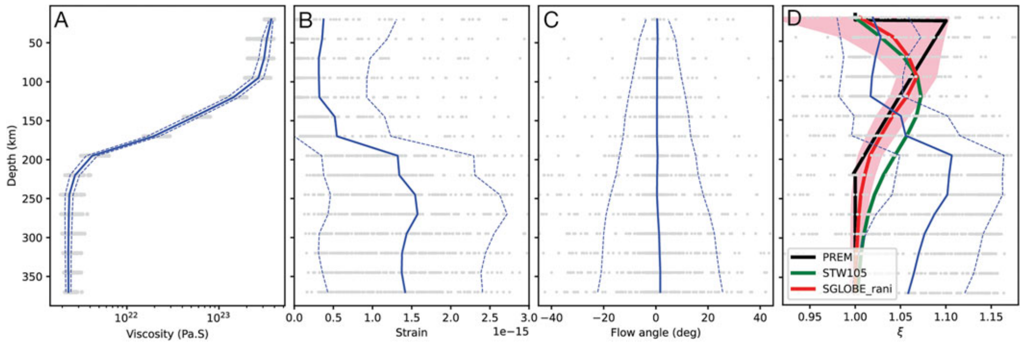

Figure 6. Depth-averaged radial anisotropy predicted by the example MCM. (A–C) The most relevant parameters to the generation of upper mantle anisotropy for the final time step of the model (using [68]). The imposed viscosity structure (A) in the uppermost mantle comprises a high-viscosity lid, with a two orders of magnitude reduction occurring between 70 and 220 km. The lid surface is driven by the imposed plate velocities. The greatest vertical gradient in velocity—and hence strain—occurs in the lower viscosity region peaking approximately 250 km (B). The model is dominated by horizontal flow (flow angle equals zero) throughout the upper mantle (C). (D) The predicted radial shear-wave anisotropy (ξ, blue line) associated with this flow structure, compared with a global averages from PREM [41] (black line) and STW105 [69] (green line), and average and standard deviation from SGLOBE_rani ([60], red line and pink shading, respectively). In all panels, grey dots show the individual points, where the model is evaluated, the solid blue line shows the average and the dotted lines the standard deviation for the MCM. It is clear that while this MCM predicts $\xi > 1$—and a comparable magnitude—of radial anisotropy, it is much deeper than observed.

with observation (in this case with PREM [41], STW105 [69] and SGLOBE_rani [60]) shows that the shear-wave radial anisotropy has the same sense (i.e. $V_{\mathrm{SH}} > V_{\mathrm{SV}}$) and similar magnitude as that measured for the Earth. This is consistent with an upper mantle dominated by horizontal flow, and lattice-preferred alignment of olivine and enstatite. However, for the tested MCM, the anisotropy magnitude peaks much deeper than for the Earth (approx. 250 km, rather than in the upper 150 km). As demonstrated in figure 6, this is a consequence of the shallow viscosity structure of the example MCM that acts to concentrate strain below the thick high-viscosity lid and also the effects of anisotropy 'frozen' in deep cratonic roots on the reference models. Models for which an Earth-like shallow flow regime is a priority would need to include a much thinner high viscosity 'lithosphere' so that strain is concentrated at shallower depths. Note that, we have not included here the effect of tomographic filtering (e.g. [70]), which would be needed for more quantitative comparison.

If the detail of shallow mantle flow is the objective of the model, then comparisons with upper mantle anisotropy can be extended. Three-dimensional tomographic models of radial anisotropy (e.g. [58–60]) could be compared globally or regionally depending on the target of interest. The assumption of radial anisotropy could be relaxed, and a more general azimuthal style of anisotropy could be compared with models derived from surface waves (e.g. [71,72]) or SKS/SKKS phases (e.g. [73]) for better resolution of the flow, at the cost of accounting for significantly more parameters.

(ii) Phase velocity maps

Surface waves provide the strongest constraints on upper mantle structure. We can thus test the global upper mantle structure of the MCMs using both measurements (e.g. phase velocity maps) and tomography models (discussed in the next section). In either case, it is vital to have a good handle on the data uncertainties.

Here, we build global fundamental mode phase velocity maps up to degree approximately 40 using the phase velocity data obtained by Ritsema *et al.* [49]. This dataset includes approximately 13 M measurements that cover 17 period bands (38–275 s). Since depth sensitivity increases with period, our data are sensitive to the whole uppermost mantle down to approximately 300 km (electronic supplementary material, add fig. S6). Data errors are estimated using a cluster analysis, the inversions are weighted using ray path density and model errors are computed from the model covariance matrix (for details about the inversions, see electronic supplementary material, S3.2.2).

We use MINEOS [74] to predict phase velocity maps using a series of one-dimensional profiles extracted from the MCM on a $2 \times 2°$ grid. We use all the 17 period bands for which real data are available and fix the crust to CRUST1.0 [75]. This ensures that realistic crustal properties are used in the comparisons. A tomographic filter (see §4a(ii)) obtained using the real phase velocity maps is applied to the predicted maps to account for the ray coverage, parameterization and the regularization applied. This allows us to calculate a quantitative misfit between the real and predicted phase velocity maps at each period; see electronic supplementary material for details.

Comparisons of the predicted MCM phase velocity maps with the observed seismic phase velocity maps are shown in figure 7. We compute overall misfits for each map and for all wave periods (figure 7e), as well as geographically for $T \sim 50$ s, $T \sim 100$ s and $T \sim 150$ s (figure 7d). The overall misfit plot (figure 7e) shows a general trend of decreasing misfit with increasing wave period, thus indicating the largest differences between the models occur in the shallow mantle (see electronic supplementary material, fig. S6 with sensitivity kernels showing that the sensitivity depth increases with increasing period). This may be due to limitations in CRUST1.0 as well as in the shallow structure predictions from the plate model used to build the MCM. Moreover, figure 7e also shows the largest misfits along major subduction zones. This could be due to the simplified lithosphere or limitations in the modelling of the shallow subduction in the MCM, which is further discussed in the next section. Furthermore, we emphasize that the main purpose of this study is to provide a tool to test MCMs, with the MCM used being just an illustrative example.

While figure 7 shows comparisons to fundamental mode Rayleigh phase velocity maps, the analysis can be further extended in future work to include comparisons with overtones. Overtones have greater sensitivity with depth, allowing us to investigate mid-mantle structure (down to approx. 660 km depth). Further comparisons can also be made with Love wave phase velocity maps, which have a different sensitivity, and to group velocity maps.

(iii) Surface wave tomography

Seismic data collected in oceanic regions are noisy and have poor coverage. This leads to surface-wave tomographic models with complex three-dimensional resolution and uncertainties. To account for these, here we use the tomographic model *SOLASW3DPacific* [76] built using the SOLA inverse method [77–80] within a finite-frequency framework [81]. The SOLA method provides control over the tomographic resolution (guaranteed to be amplitude bias-free) and uncertainty. By construction, it produces all this information at no extra computational cost. In addition, the finite-frequency framework allows the surface-wave tomography model, and its resolution, to be fully three-dimensional.

Here, we assess the predicted three-dimensional V_{SV} of the MCM in the Pacific upper mantle. The predicted structure, obtained from the conversion of MCM outputs using mineralogical models described above and initially provided on a very fine grid is interpolated on to the coarser tomographic grid ($2 \times 2°$ laterally and 25 km vertically). We apply the SOLA resolution matrix, before we compute the misfit with the data-based tomography model accounting for tomographic uncertainty. Further details are given in the electronic supplementary material, S3.3.

Similar to the previous section, we find that away from subduction zones there is good agreement between the MCM prediction and the SOLA model at a depth of 112 km (figure 8): both show the low-velocity mid-oceanic ridges, high-velocity cratons and a smooth increase of velocity with distance from the ridge. In subduction zones, the agreement is poor: while the MCM predicts high velocities corresponding to plunging slabs, the SOLA tomography model shows low velocities in these regions.

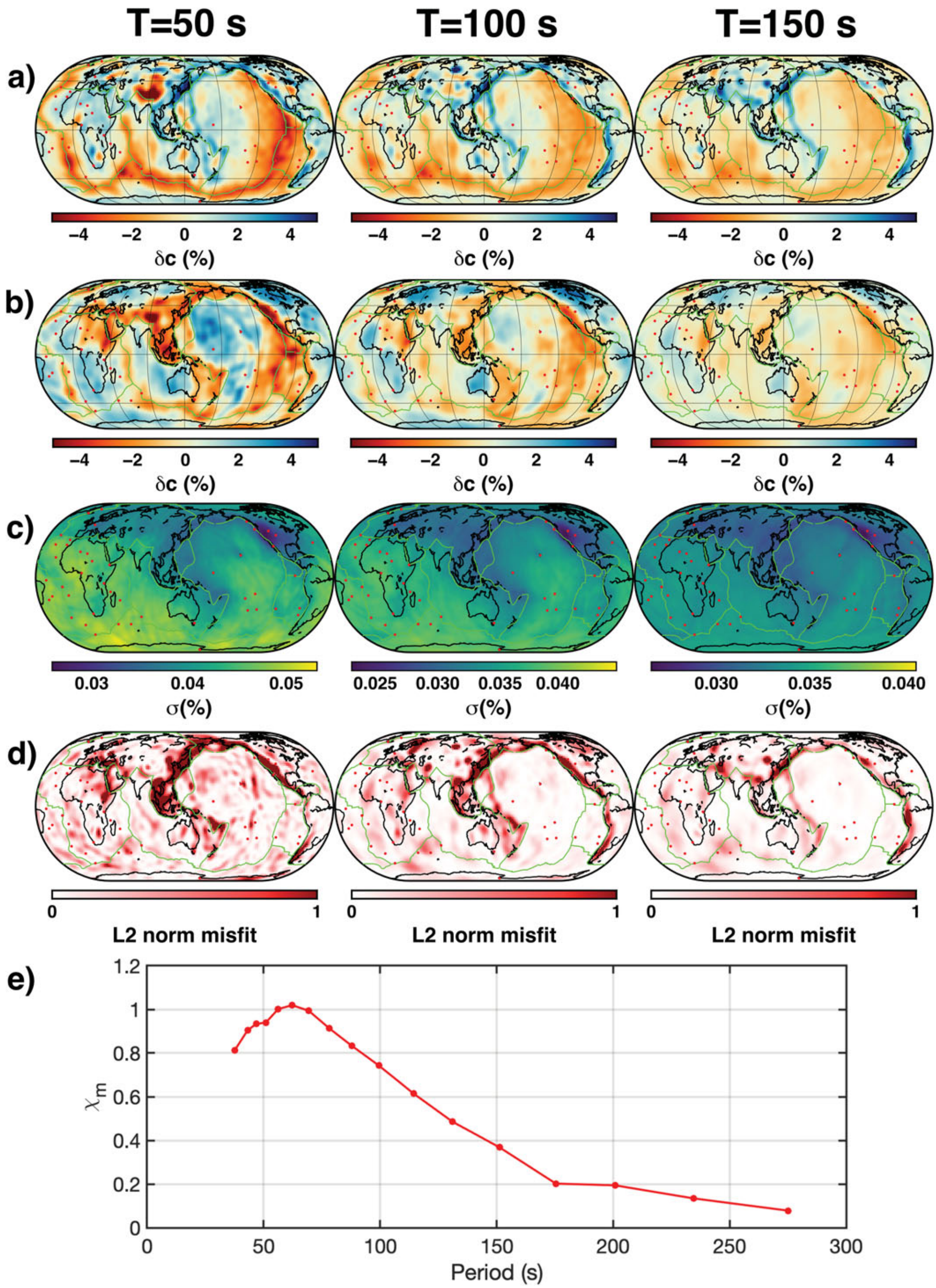

Figure 7. (a) Predicted phase velocity perturbations for the example MCM, with a tomographic filter based on the measured phase velocity maps applied. (b) Real phase velocity maps from Rayleigh wave measurements. (c) Associated phase velocity error maps. (d) Geographical L2 norm misfit maps. (e) Global misfit as a function of period. All maps are shown at three illustrative periods of 50, 100 and 150 s.

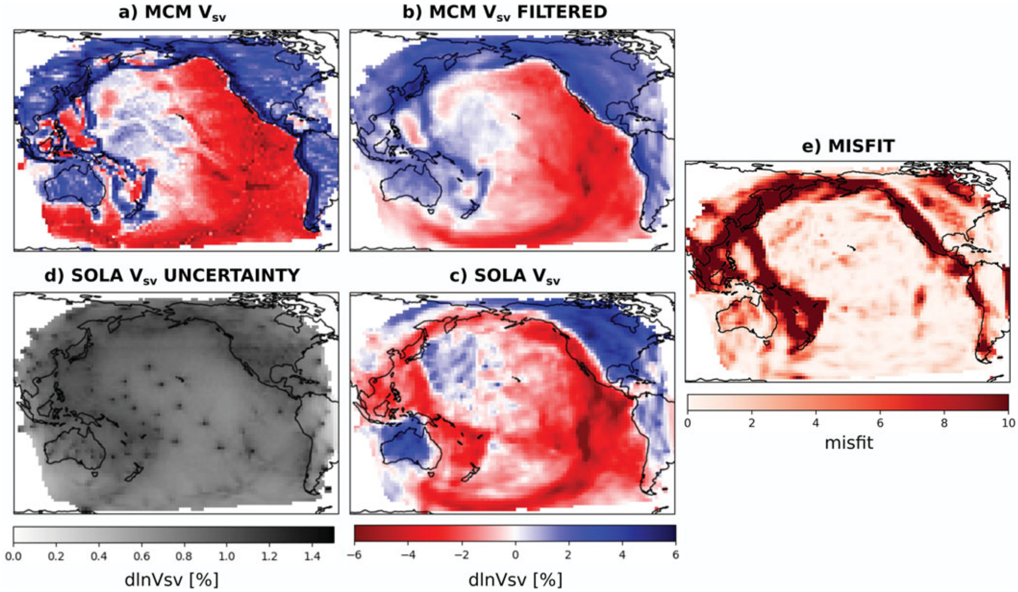

Figure 8. (a) V_{SV} structure predicted by MCM, interpolated on to the tomographic grid, and (b) filtered with SOLA resolution. (c) Data-based SOLA V_{SV} tomography model and (d) uncertainty. (e) Misfit (in multiples of SOLA model uncertainty). All maps are at 112 km depth.

There are several possible explanations for this discrepancy. (i) The lithospheric structure is overly simplified in the MCM—particularly, the ocean-continent dichotomy is not modelled; (ii) slab-induced circulation is not well-constrained; (ii) low-velocity anomalies at subduction zones in tomography models are often interpreted to be due to hydration melting, [82] a process not modelled in the MCM. (iii) We can perhaps observe the slab signature in SOLA, but it is far weaker than in the MCM. One explanation is that the slabs are too thick in the MCM or, produce too strong anomalies, or do not have the right geometry. Alternatively, this could be due to lateral leakage effects due to the resolution, even if the MCM has been filtered by the SOLA resolution. In the SOLA model, low-velocity anomalies due to hydration melting may mask the slab signature, but this does not happen in the MCM where hydration melting is not modelled. These discrepancies hold for this specific MCM where the shallow structure appears to be overly simplified. This is a motivation to use more realistic shallow mantle structure in future MCMs and to account for hydration melting.

During these comparisons, we must be aware that the tomographic models are not perfect. Even though we account for their limited resolution and uncertainty, errors due to theoretical approximations are not accounted for [76]. In particular, the strong misfit in Western North America might be explained by nonlinear effects not accounted for in the tomography model rather than weaknesses in the MCM. See the electronic supplementary material for other possible seismic constraints.

5. Testing models with magnetic observations

The geomagnetic field is generated via a dynamo process in Earth's liquid iron outer core, in which thermal and compositional convection drives motion of an electrically conducting fluid. The field is thought to have been dipole-dominated for most of its history [83] and undergoes spontaneous polarity reversals, in which the positions of the north and south magnetic poles are swapped over a period typically lasting thousands of years [84]. The reversal frequency has varied from the present-day average value of three to four reversals every million years, to less than one reversal per 10 million years during the Cretaceous Normal Superchron (CNS) and Kiaman Reverse Superchron (KRS), to more than 10 reversals every million years during hyperactive periods such as the mid-Jurassic [85], Early Carboniferous [86] and Ediacaran-Cambrian [87].

Several studies have linked variations in reversal frequency to variations in mean CMB heat flux Q, as well as the amplitude and pattern of heat flux heterogeneity [88–95]. The relationship between reversal frequency and CMB heat flux variations is suggested by numerical dynamo simulations. These simulations consistently show that increasing the buoyancy force powering core convection with all other control parameters fixed drives the dynamo from a state in which the CMB field is strong, dipolar and non-reversing to a state in which the CMB field is weak, multipolar and frequently reversing [96–100]. Dipolar reversals tend to lie near this dipole-multipole transition, suggesting that Earth's core may also lie close in parameter space to this transition [98], thus explaining the periods of both low and high reversal frequency as the field fluctuates between either side of this regime. As explained below, when testing our MCM based on magnetic observations we have investigated Q over the last approximately 300 Myr, during which time the outer core has had a thick-shell geometry and all of the dynamo control parameters other than buoyancy driving have been essentially constant [101]. Hence, changes in buoyancy (and hence Q) are expected to be the main factor determining the rate of reversals. We would expect changes in Q in our MCM over the last 300 Ma, where short-term fluctuations are controlled by variations in the temperature at the CMB, the temperature at the top of the thermal boundary layer and the thickness of the boundary layer itself.

The direct relation between a given value of Q and a given reversal frequency, or indeed the amplitude of Q at which reversals are induced, is unknown. Ideally, one would consider the connection between CMB heat flux and reversal frequency directly by investigating an MCM coupled to numerical dynamo simulations. However, given that dynamo simulations cannot be run at the physical conditions of Earth's core and that multiple computationally expensive simulations would be required to simulate different times in Earth's history predicted by a single MCM, such an investigation would require its own systematic study. We seek criteria that can be applied to any MCM and therefore base our constraining observation solely on the fact that higher Q generally corresponds to more reversals, with periods of high reversal frequency caused by high Q, and periods of low reversal frequency caused by low Q. Comparing Q in our MCM to the reversal frequency inferred from paleomagnetic observations can therefore be used to constrain lower mantle heat flow over time (figure 1).

Since both the heat flow and reversal frequency are not well-constrained, rather than calculating a correlation coefficient in the manner of Choblet *et al.* [102], we instead consider the variation of heat flow properties averaged over the present-day (P, 0–25 Myr), the mid-CNS (CNS, 90–110 Myr) and the mid-Jurassic (J, 150–170 Myr). Although future work could use the methodology proposed in this paper to better constrain the heat flux at the CMB, current estimates range from 5–15 TW and as such we do not put any emphasis in our criteria on the value of the heat flux itself, instead comparing the ratios of the average heat flow over the aforementioned time periods. Heat flow should be higher at present-day and during the Jurassic than during the CNS, and as such an MCM should satisfy the ratios

$$\frac{Q_P}{Q_{\mathrm{CNS}}} > 1 \quad \text{and} \quad \frac{Q_J}{Q_{\mathrm{CNS}}} > 1, \tag{5.1}$$

indicating that over the past 170 Myr the heat flow declined and then rose again. When applying our chosen ratios to the MCM, we find that $Q_P/Q_{\mathrm{CNS}} = 0.988$ and $Q_J/Q_{\mathrm{CNS}} = 0.962$ giving the model a score of 0 out of 2 for this criterion.

While not part of our criteria, we also consider the amplitude of the CMB heat flux heterogeneity $Q^* = (Q_{\max} - Q_{\min})/2Q$, since larger Q^* indicates locally stronger core convection that could induce reversals, and hence we would expect Q^* to satisfy the same ratios as Q. For the MCM considered here, the time-averaged Q^* is higher during the CNS compared with the Jurassic and present-day, and hence would not satisfy any criteria based on ratios of Q^*; Q^* does not significantly vary throughout the 170 Myr (with a standard deviation of 0.03 compared with that of 0.18 for Q), indicating it may not be particularly useful for verifying the validity of this model regardless of the ratios.

We also investigated the evolution of the spherical harmonic component Y_2^0, where positive and negative values correspond to large equatorial and polar heat flux, respectively. Equatorial cooling is thought to induce reversals even if Q is low [103], while enhanced polar flux stabilizes the dipole [90], hence Y_2^0 would ideally be negative during the CNS and positive during the Jurassic and present-day. We find for this model that Y_2^0 is negative throughout the period from 170 Myr to present, with the dipole most stabilized during the CNS, indicating that there is no increased equatorial heat flux that would influence the reversal frequency in this case.

We chose to use only the ratios Q_P/Q_{CNS} and Q_J/Q_{CNS} for our geomagnetic metrics as plate tectonic models are better constrained from 170 Myr onwards, leading to the exclusion of ratios involving the KRS. For this model, if we were to consider the heat flux during the Kiaman Q_{KRS} (averaged over 312–262 Ma), we find that $Q_P/Q_{\mathrm{KRS}} = 1.031$ and $Q_J/Q_{\mathrm{KRS}} = 1.004$. This is in contrast to the CNS ratios. Another ratio that could be considered is Q_J/Q_P, which given the reversal hyperactivity during the Jurassic we would also expect to be greater than one. We chose to omit this ratio from the geomagnetic criteria to focus solely on whether Q falls before then rising after the CNS. We find $Q_J/Q_P < 1$ and hence would not result in this model achieving a higher rating if we did choose to consider three ratios rather than two.

6. Testing models with dynamic topography and geoid observations

(a) Observations

A variety of independent estimates of Earth's surface and CMB deflections can be used to test predictions from MCMs. Since the simulations we examine, like many others, incorporate forcing by horizontal plate motions, we focus on comparing predicted vertical deflections at Earth's surface, h. Arguably the most direct observational evidence for vertical motion induced by mantle convection arise from residual oceanic age-depth measurements, observations of uplifted marine rock and subsidence patterns that cannot be explained by tectonic (e.g. shortening, extension, flexure), glacio-eustatic or sedimentological processes, e.g. [8,9,104] and references therein. A variety of other indirect estimates including uplift histories from inverse modelling of geomorphic geometries, hiatus mapping and geochemical palaeoaltimetry can also provide information about histories of surface deflections generated in response to mantle convection, e.g. [105–107] (schematically represented in figure 1). This summary of observations is necessarily very brief; the interested reader is directed to [8,9,108] for a more detailed introduction to the topic. Independent estimates of dynamic topography at the CMB are more equivocal and we do not explore them further in this contribution, e.g. [109].

It is straightforward to compare deflections predicted by different simulations. In the following section, we first summarize methodologies we have used to generate predictions of dynamic topography from MCMs, with a focus on aiding comparison to a variety of observations and predictions. We then summarize approaches used to assess similarities and differences between predicted surface deflections and independent estimates. An extended description of these methodologies and associated mathematics are provided in the electronic supplementary material.

(b) Testing predictions

Perhaps the harshest test of surface deflections predicted by a mantle convection simulation is to calculate Euclidean (e.g. root-mean-squared, χ; see eqn. (16) in electronic supplementary material) misfit between the predicted surface (or derived quantities, e.g. rates of change) and independent estimates. Surface deflections, h, can estimated from MCMs by requiring normal stresses to be continuous across the upper boundary of the solid Earth and the (assumed) overlying fluid with density ρ_w, such that $\sigma_{rr} + \rho_m g_s h = \rho_w g_s h$, where σ_{rr} incorporates the deviatoric viscous stresses generated by mantle convection and dynamic pressure, ρ_m is mean density of the surficial layer of the model and g_s is gravitational acceleration at Earth's surface, e.g. [110,111]. Once armed with such estimates of surface deflections it is straightforward to compare them to independent (gridded or spot) estimates, e.g. [104,112]. However, such estimates tend to be extremely sensitive to noise and misalignment, e.g. [113]. We might, instead, be interested to know whether a simulation predicts surface deflections with broadly the correct frequency content. For instance, it might be useful to know if a simulation has broadly the correct number of upwellings and downwellings at the correct scale. By transforming surface deflections into the spherical harmonic domain, predictions and independent estimates can be compared at appropriate scales and their power spectra can be assessed, e.g. [8,114].

An alternative approach is to calculate surface deflections using the analytic propagator matrix technique. This approach requires the generation of sensitivity kernels that relate density anomalies in the mantle to surface deflections, e.g. [111,115,116]. The kernels principally depend upon (radial) viscosity and boundary conditions. A fuller mathematical description is given in electronic supplementary material. There exists a variety of methodologies to establish similarities and discrepancies of predicted surface deflections with independent estimates once surface deflections are in the frequency domain. First, the degree correlation spectrum, r_l, provides estimates of correlation between independent estimates of dynamic topography and predictions from simulations for each spherical harmonic degree, l, see eqn. S17 in electronic supplementary material, [11]. It is straightforward to calculate the mean value, i.e. $\bar{r}$. Second, the correlation of the entirety of the two fields being compared can also be straightforwardly estimated in the frequency domain, r, see electronic supplementary material, eqn. S18, [11]. This metric is not, however, sensitive to the amplitudes of the fields. Finally, once armed with spherical harmonic representations of the fields being compared, it is straightforward to generate and compare their power spectra, ϕ, or compare power spectra to other independent estimates, e.g. Kaula's rule, see electronic supplementary material, eqn. S19 [8].

It is also straightforward to compare the geoid predicted from MCMs and independent estimates. Similar to the treatment of dynamic topography, these comparisons are performed in the frequency domain. The geoid is estimated by combining the calculated density structure from the MCM with a geoid sensitivity kernel (see electronic supplementary material). We assume free-slip boundary conditions at the surface and CMB (i.e. vertical velocities = 0, horizontal velocities are free to vary). The degree correlation, correlation of the entire fields and power spectra can now be calculated to compare the predicted geoid with independent estimates, e.g. from satellite altimetry. Here, we compare results to EIGEN-5C [117,118].

(c) Results and suggested improvement

While in principle the topography comparisons can be done over recent geological history, we focus here on comparisons at the present day. Figure 9 shows surface deflections calculated using present-day densities predicted by the MCM and the propagator matrix technique to compared independent estimates of dynamic topography up to degree 30. It summarizes the assessment of their similarities and differences; χ_p annotated in panel c was calculated by comparing surface deflections predicted using the entirety of the MCM domain (i.e. from the CMB to the surface), Kaula's rule (thin grey curve) and an estimate of residual topography from [8]. In these examples, we assume that the fluid overlying the solid Earth is water with $\rho_w = 1030\,\mathrm{kg\,m^{-3}}$. The associated values for models in which the uppermost 100 km (dashed) and 300 km (dotted) of the model domain are excised are $\chi_p = 8.7$ and $\chi_p = 7.2$, respectively. These results, combined with visual inspection of panels a and b, demonstrate that surface deflections from the MCM tend to over-estimate independent estimates of dynamic support by at least an order of magnitude even when the uppermost 100 km of the model domain is excised. Increasing the depth of excision to 300 km brings calculated power spectra nearer to that of oceanic age-depth residuals, but it over-steepens the spectral slope. Consistent with these results, histograms showing the distribution of amplitudes, calculated χ and correlation coefficients, r, r_l and $\overline{r_l}$ (see annotations on figure) emphasize a lack of similarity between the models at nearly all degrees. In nearly all places and all scales the MCM tends to have larger (positive and negative) amplitudes than the independent estimates. Similarly, the MCM tends to over-predict the amplitude of the geoid.

A straightforward addition to this work would be to compare histories of predicted surface deflections and polar wander to independent observations, e.g. [108,112,119]. There are a number of outstanding challenging issues associated with determining contributions to surface deflections from the convecting mantle, not least disentangling lithospheric contributions, e.g. [8,110,120]. It is relatively straightforward to separate deflections generated by loading and flexure of the lithosphere by focusing on deflections at wavelengths longer than even the strongest lithosphere can support elastically, e.g. [8,121]. Here, we consider deflections at spherical harmonic degrees $l \leq 50$, which, at Earth's surface, includes wavelengths, $\lambda \gtrsim 793$ km ($\lambda \approx 2\pi R/\sqrt{l(l+1)}$, where $R \approx 6370$ km is Earth's radius [122]). A much more difficult problem is isolating dynamic support from lithospheric isostasy, e.g. [123]. A variety of techniques exist to do so, perhaps the most widely used approach is to simply not include the shallowest few hundred kilometres of the model domain in calculations of surface deflections, as we have explored, e.g. [7,112]. However, this approach can also excise contributions from the shallow convecting mantle, which is undesirable because of surface deflection sensitivity to density anomalies in the uppermost convecting mantle, e.g. sensitivity kernels in [111,115,116,124], which depend on assumed radial viscosity. Alternative approaches include removal of lithospheric isostatic contributions using independent information about its structure derived from, for instance, shear wave tomographic models [125,126]. Perhaps the most obvious opportunities to improve predicted surface deflections from numerical simulation include allowing surfaces to deform, self-gravitation, development of a probabilistic understanding of mantle circulation and resultant effect on surface deflection uncertainties, and incorporating better understanding of lithospheric structure, especially of lithospheric densities, viscosity, and thermal boundary-layer evolution. Many of these issues are actively being addressed, e.g. [9] and references therein.

7. Testing models with geochemistry and petrology

Three geochemical/petrological metrics are used to rate MCMs: (1) examining how attributes of MCM particles (which track chemistry) beneath ridges and plumes compared with the results of a geochemical model quantifying mantle source parameters from measured mid-ocean ridge basalts (MORB) and ocean island basalts (OIB) radiogenic isotope data (Sr, Nd, Hf, Pb); (2) comparing the Th/U and ^{238}U/^{235}U values of MCM particles to modern day measured MORB and OIB values following the recycling of excess U relative to Th and of ^{238}U relative to ^{235}U into the mantle; (3) comparing estimates of temperatures of OIB and MORB source regions using petrologic geothermometers versus MCM predictions. Note that, the first two metrics have the ability, in principle, to sense changes over time, while the third is potentially a direct estimate of a driver of mantle circulation, i.e. thermal buoyancy (figure 1).

(a) Testing models against a geochemical inversion of MORB and OIB radiogenic isotope data

Evidence for mantle compositional heterogeneities have long been identified from the radiogenic isotope systematics of MORB and OIB (eruptive products of mantle plumes) [127,128]. Systematic isotopic differences require long-lived chemical heterogeneities, consistent with varying extents of radiogenic ingrowth from distinct parent/daughter isotope ratios [129]. The recycling of mafic crustal material into the mantle exerts a primary control on these heterogeneities as it is several orders of magnitudes more concentrated in radioactive and radiogenic trace elements compared with mantle peridotite [130]. On average, OIB show more chemically enriched radiogenic isotope signatures compared with MORB (higher ^{87}Sr/^{86}Sr, ^{206,207,208}Pb/^{204}Pb, lower ^{143}Nd/^{144}Nd,

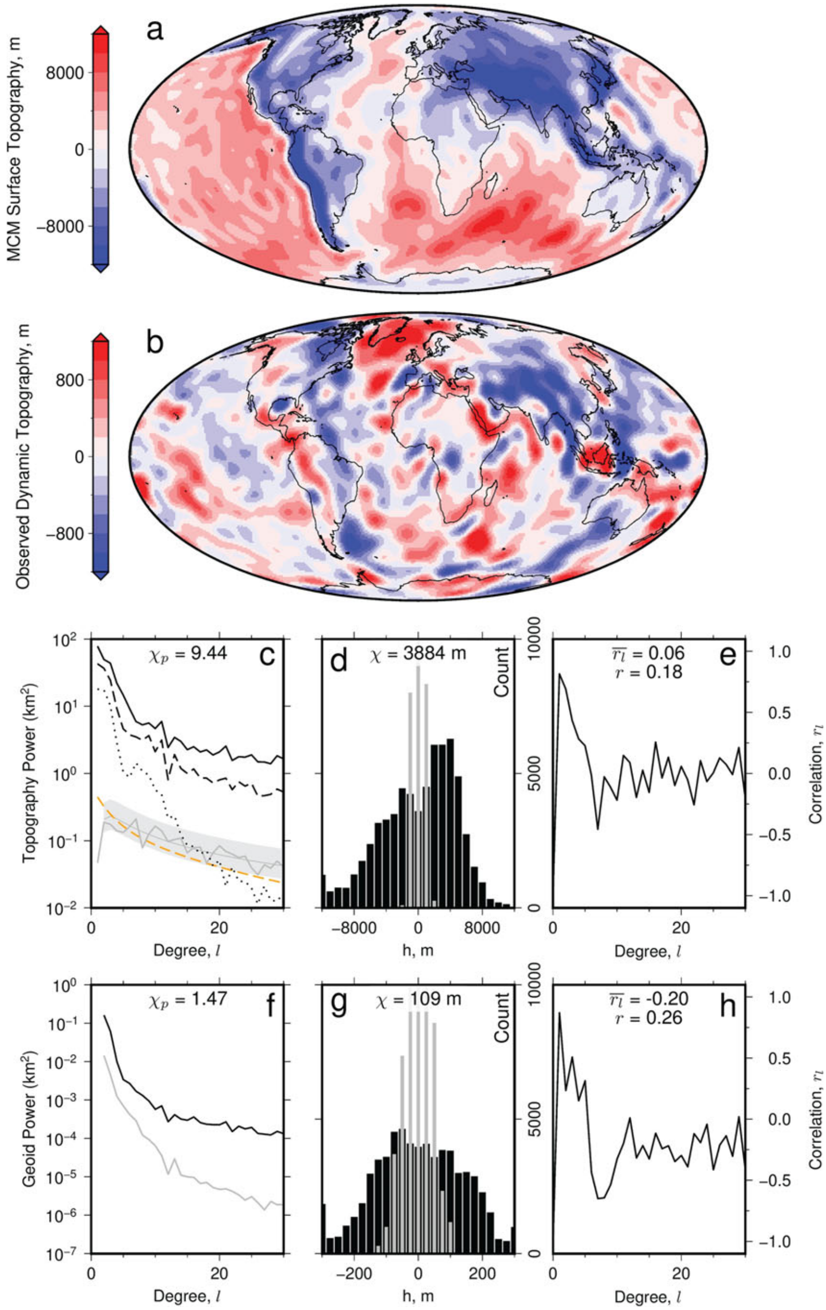

Figure 9. Comparison of modern surface deflections and the geoid predicted by MCM with independent observations up to $l = 30$ (see body text for details). (a) Water-loaded surface deflections predicted by MCM. (b) Calculated residual topography from [114]. (c) Solid black = power spectrum of topography shown in a. Dashed and dotted black = spectra when the uppermost 100 and 300 km of the MCM are excised, respectively. Thin grey curve and band = expected dynamic topography from Kaula's rule using admittance $Z = 12 \pm 3$ mGal km^{-1}. Thick grey = power spectra of residual topography shown in b. Orange dashed = expected power spectra for water-loaded residual topography from [8]. (d) Black/grey = histograms of amplitudes shown in a/b. (e) Spectral correlation coefficients, r_l, for a and b. (f) Black = power spectrum of geoid calculated using TERRA. Grey = Eigen5c [117]. (g) Black/grey = histograms of geoid amplitudes in MCM/Eigen5c models. (h) Correlation coefficients for MCM/Eigen5c. Note annotated values of χ_p, χ, $\overline{r_l}$ and r are discussed in the body text.

^{176}Hf/^{177}Hf), suggesting larger amounts of recycled crust in the source of mantle plumes compared with the mid-oceanic ridge mantle.

Plumes sample the deeper mantle [131] and crustal material is more dense than mantle peridotite across most mantle depths [132,133]. The relative enrichment of plumes in crustal material compared with the surrounding mantle sampled by mid-oceanic ridges is quantitatively limited by the buoyancy of ascending crustal material, which can be varied across MCMs by adjusting the buoyancy number of the basalt. MCM particles keep track of crustal material circulating in the mantle (through the *C* attribute). The mean difference in the amount of crustal material between the mantle melting at plumes and ridges in MCMs can therefore be directly compared with the same metric derived from Earth's MORB and OIB radiogenic isotope dataset. This comparison allows for an evaluation of whether assumptions about the buoyancy of crustal material in the MCMs are Earth-like.

Quantifying the enrichment in crustal material of plumes (OIB source) relative to ridges (MORB source) from real MORB-OIB radiogenic isotope data is not straightforward. This is because the amount of crustal material in the mantle is one of many parameters controlling the radiogenic isotope composition of mantle-derived basalts [129,134]. We address this problem in a geochemical model (see details in electronic supplementary material) where we explore the detailed geochemical parameter space of mantle source evolution leading to modern basalts from a primitive mantle source at 4.57 Gyr. Parameters of this model include the extent of peridotite melt-depletion, the amount of crustal material recycled into the mantle, the ages of source modification, the proportion of continental material, and the alteration/dehydration of crustal material. We interpret global radiogenic isotope datasets for MORB and OIB (from the GEOROC and PetDB databases) with this model on a sample-to-sample basis through a *Monte Carlo* approach. Results of our geochemical inversion yield a mean amount of crustal material $f_{\mathrm{RC}}^{\mathrm{OIB,Geochem}} = 7.0\%$ in the OIB source, and $f_{\mathrm{RC}}^{\mathrm{MORB,Geochem}} = 5.7\%$ in the MORB source. This means the difference in crustal material enrichment of the OIB source relative to the MORB source is $\Delta f_{\mathrm{RC}}^{\mathrm{Geochem}} = +1.3\%$. Note that, the mean OIB value is weighted by the buoyancy flux of individual plumes [120] rather than by the number of samples.

To make the same comparison with the MCM, we extract the particles present under ridges and plumes active in the MCM at present day. Particles located right under the melting zones are selected to ensure their *C* values reflect time-integrated chemistry rather than present-day melting. Particles are associated with a ridge if they lie laterally within 75 km of the ridge axis as it is projected vertically down into the mantle in a depth range of 135–300 km. To identify plumes, we use the plume detection scheme implemented in terratools [68] which uses the product of the non-dimensionalized radial velocity and temperature fields (electronic supplementary material, S5.1). Particles are associated with plumes if they fall within the bounds of any of the identified plumes in depth range of 135–300 km (electronic supplementary material, S5.1). The f_{RC} value are calculated from the *C* values of populations of particles (one f_{RC} value per population), using electronic supplementary material, eqn. SM.23.

Particles under plume melting zones are grouped into a OIB source population yielding $f_{\mathrm{RC}}^{\mathrm{OIB,\,MCM}}$. All particles under ridges are grouped into a MORB source population yielding $f_{\mathrm{RC}}^{\mathrm{MORB,\,MCM}}$. The enrichment in crustal material of plumes relative to ridges $\Delta f_{\mathrm{RC}}^{\mathrm{MCM}}$ is then the difference between the two values. The MCM yields a $\Delta f_{\mathrm{RC}}^{\mathrm{MCM}}$ of +1.1% with an inter-plumes standard deviation of ±1.2%, thus near-identical to $\Delta f_{\mathrm{RC}}^{\mathrm{Geochem}} = +1.3\%$.

(b) Testing models with Th/U ratios and U isotopic compositions of mantle-derived basalts

Following the onset of the first major rise in atmospheric oxygen across the great oxygenation event (GOE) (approx. 2.3 Ga), there would have been a supply of continent derived U to the oceans due to oxidative weathering. The hydrological recycling of this U relative to Th (which is fluid immobile) from the continental crust into the upper mantle, through subduction, can result in the lowering of the upper mantle Th/U, measured in MORB, faster than the time integrated

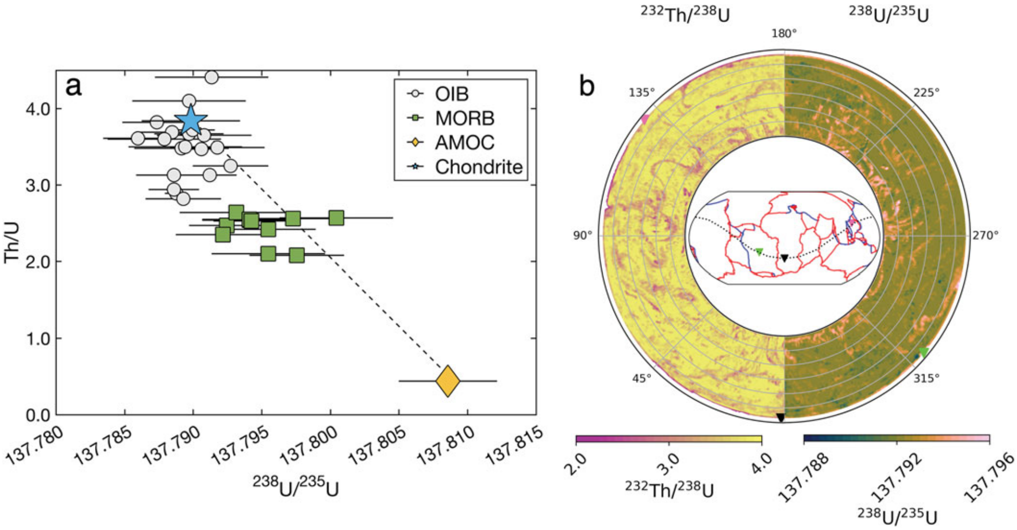

Figure 10. Overview of U elemental and isotopic recycling in MCM runs (a) Uranium isotopic compositions, $^{238}U/^{235}U$, versus Th/U ratio for mantle derived basalts, chondrite and AMOC. Figure is re-created and modified from [140]. Ocean island basalts (grey circles) have similar $^{238}U/^{235}U$ to chondrite (blue star), while the higher $^{238}U/^{235}U$ and lower Th/U of MORB (green squares) imply a mixture (black dashed line) between chondrite and AMOC (yellow diamond), represented by the Ocean Drilling Program site 801 Supercomposite. Data are from [140] and error bars are the two standard error. Isotopic data has been converted from δ notation to ratios by normalizing to a $^{238}U/^{235}U$ ratio of 137.832 [140]. (b) Global cross section for the example MCM following 1.2 Gyr of excess U recycling relative to Th and 0.7 Gyr of excess ^{238}U recycling relative to ^{235}U showing (left section) $^{232}Th/^{238}U$ and (right section) $^{238}U/^{235}U$ at 0 Ma, with an inset map showing red and blue lines for locations of ridges and subduction zones, respectively, and dotted black line with coloured triangle indicating the direction of the cross section.

Th/U ratio calculated from Pb isotopic compositions of MORB [135–137]. The gradual lowering of the Th/U ratio of the upper mantle from chondritic compositions (approx. 3.9) [138] since the GOE to compositions measured in modern day MORB (approx. 2.4–3.8) [139] reflects the pollution of the upper mantle with surface-derived, recycled U (figure 10a). Ocean island basalts also show a range in largely sub-chondritic Th/U ratios (approx. 3–4.5), that reflect recycled U, but are typically higher than MORB (figure 10a). A positive trend between Pb model ages of OIB sources and their Th/U ratios [140,141], reflects the continual recycling into lower mantle OIB sources of crust produced from an upper mantle with steadily decreasing Th/U. Therefore, the recycling of U generates distinct patterns in U elemental geochemistry across the mantle that can be used to assess MCMs.

The isotopic behaviour of U also provides a complement to the inferences that can be gained from elemental Th/U. Low-temperature isotopic fractionation of U during hydrothermal seawater alteration of the oceanic crust and associated uptake and enrichment of U results in low Th/U and isotopically distinct $^{238}U/^{235}U$ ratios of altered mafic oceanic crust (AMOC), that are on average elevated above chondritic compositions [140] (figure 10a). Mid-ocean ridge basalts have low Th/U ratios and higher $^{238}U/^{235}U$ ratios than chondritic compositions that are attributed to the pollution of the MORB source with recycled isotopically distinct AMOC [140] (figure 10a). Ocean Island basalt sources, however, have chondritic $^{238}U/^{235}U$ ratios, which is inconsistent with the modern U cycle [140] (figure 10a). Given the redox sensitive nature of U, the high $^{238}U/^{235}U$ ratios of AMOC is a recent feature in Earth's history; the isotopic fractionation during the alteration of ocean crust has probably only occurred since the deep oceans became oxygen rich [140] (approx. 0.8–0.4 Ga, e.g. [142–145]). Therefore, OIB and MORB sources appear to be differently polluted by recycled oceanic crust, with more and isotopically distinct U returned to the shallow MORB source than deep OIB sources. This is another distinct mantle geochemical parameter that can be used to assess MCMs, and notably the responsible process has a 'known' start time of approximately 0.8–0.4 Ga, within the time-period of the MCM.

The MCM started with set initial concentrations of U and Th and recycled a set excess flux of U relative to Th into the mantle over 1.2 Gyr of convection (see [146] for an example of U recycling in MCMs). By monitoring the ratio of ^{232}Th and ^{238}U particles over the time scale of convection we can compare the ratios in plumes relative to those under ridges, to examine how well they reflect present day measured values of OIB and MORB, and the relative differences between the two groups of mantle derived basalts (figure 10b). From 0.7 Ga (our chosen time of deep ocean oxygenation) the MCM preferentially recycles 0.02% more ^{238}U relative to ^{235}U, compared with the chondritic Earth value. As a first model, this is done simply, by spreading this excess ^{238}U in the surface particles. This leads to this signature being taken deep into the mantle by subduction, which is how surface particles re-enter the convecting mantle. By comparing the ^{238}U/^{235}U ratio of plumes to ridges we can monitor the global distribution of recycled U on an ocean basin scale and compare relative differences to measurements of modern day OIB and MORB (figure 10b). However, in the MCM illustrated in (figure 10b), the expected first-order feature of lower Th/U and higher ^{238}U/^{235}U in the upper mantle, as sampled by MORB, relative to the lower mantle, as sampled by OIB, is not observed. This potentially reflects how the excess ^{238}U is recycled. It may need to be returned to the upper mantle past the zone of arc magmatism rather than be subducted into the deeper mantle by slabs, a hypothesis already proposed [140], that can be explored by further modifying the ways in which U is recycled in different MCMs.

MCMs can therefore be assessed by the relative differences in the Th/U and ^{238}U/^{235}U ratios of particles in plume and spreading centre regions (which can be done on an ocean basin scale—Atlantic, Pacific and Indian) and how well they reflect modern mantle compositions based on measurements of modern day OIB and MORB. [140].

(c) Testing models against petrological estimates of mantle potential temperature

With planetary cooling being the driver of all interior dynamics on Earth, it is natural to ask the question of whether geodynamic models are faithful to Earth's observed mantle temperature. The absolute temperature that a geodynamic model will operate at is sensitive to numerous model properties including, but not limited to, the rheology model used, core temperature, internal heating, whether boundary-layer behaviour is correctly captured and the presence and amplitude of compositional density anomalies. As a result, comparison between the absolute temperatures of models and data are unlikely to be fruitful; with model temperature adjusting according to these other parameter choices to regulate internal heating [147–149]. Instead, comparing the distribution of temperature differences within the model and within observations of Earth has the potential to remove some of these systematic offsets and illuminate the more fundamental differences in geodynamic model behaviour versus the Earth.

The natural reference temperature that connects observations and models is that of the 'ambient' mantle. On Earth, this is most readily sampled by petrological thermometers at mid-ocean ridges, where passive plate spreading causes underlying mantle to partially melt. As an MCM has the mid-ocean ridge geometry imposed upon it, then we can take the subridge regions of the model and compare the temperature of these to the temperatures reconstructed from observations.

Petrological thermometers typically do not record mantle temperature directly. We focus on using results from an olivine–spinel exchange thermometer [150,151], applied to natural basalts from mid-ocean ridges and ocean islands (results from [152]). In principle, this thermometer records the temperature at which coexisting olivine and spinel last exchanged aluminium. Given the slow diffusing nature of Al in olivine [153], this last inter-phase exchange of aluminium would have probably occurred shortly after the olivine–spinel pair crystallized from the magma (although see [151] for a discussion of how far this assumption holds). The temperature recorded by this petrological thermometer will be significantly less than the mantle temperature due to [154,155]: magmatic differentiation; adiabatic cooling of the magma during

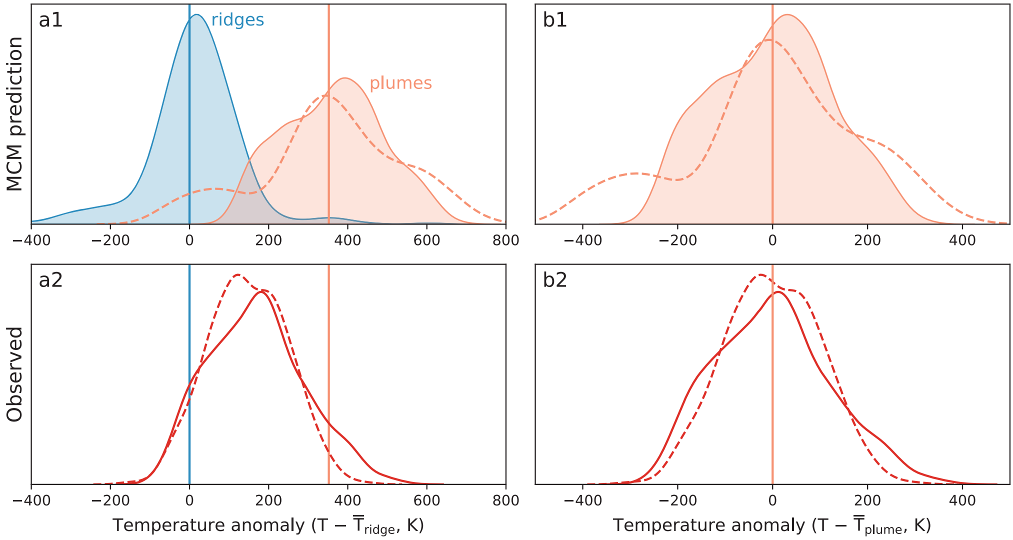

Figure 11. A comparison of MCM plume and ridge temperatures (top: a1, b1) against observed plume temperatures (bottom: a2, b2) from [156], dashed line, and [152], solid line. All temperatures are shown normalized to the ridge average temperature (MCM) or a representative ridge temperature estimate (for observationally constrained estimates). The two plume temperature distributions from the MCM results, one filled and one unfilled with a dashed line, indicate two different approaches to extracting plumes from the model: the dashed line capturing shallow mantle more likely to overlap with shallow ridge segments.

ascent; any super-liquidus cooling the melt experienced; and, cooling of the mantle during decompression melting. By accounting for these effects Li *et al.* [152] produced estimates of mantle temperature; however, it is important to note that uncertainty on the mantle temperature estimate is significantly enhanced when acknowledging the uncertain contributions to magma cooling prior to crystallization [154]. For comparison, we also include a recent compilation of mantle temperatures derived from seismology [156].

MCM temperatures for subridge mantle and mantle plumes are compared with both petrological and seismological mantle temperature estimates in figure 11. The observations of mantle temperature from both petrological [152] and estimates based on seismic tomography (corrected for tomographic filtering) [156] agree well. The MCM excess plume temperatures are systematically higher than the plume temperature excess observed on Earth by approximately 200°C on average (figure 11a1 versus a2). However, comparing the plume temperatures directly, the MCM plumes have a similar variation in temperatures to those found among ocean islands (figure 11b1 and b2). MCM plumes are therefore ‘running hot’ compared with Earth, but otherwise have the same range of hotter and cooler plumes.

As noted above, absolute model temperatures could be offset from Earth’s mantle temperature due to a wide range of model-related factors. Here, we have considered relative temperature deviations from ambient mantle to mitigate this, but still find this particular model to have hotter plumes than Earth. Hotter plumes might occur in MCMs from numerous choices made in the set-up of the simulation: whether the simulation is Boussinesq or fully compressible; the choice of rheology model; the core temperature; the bottom boundary condition, in particular the presence of dense stable piles; magnitude of compositional density anomalies (e.g. from oceanic crustal recycling); and the presence of transition zone phase changes and their associated thermodynamics.

These features of the model and parameters would need to be systematically varied to establish what choices were consistent with Earth’s observed plume temperatures. If we are then interested in accurate descriptions of intra-plate melting fluxes and chemical evolution of the mantle driven by these processes, excessively hot plumes set up a problem that is difficult to solve by adjusting the mantle’s melting properties, as that would then dampen ridge melting.

This discrepancy between petrological temperatures and model temperatures highlights the value of a multi-constraint approach to evaluating the fitness of geodynamic models.

8. Summary

We have presented a suite of observations and demonstrated how they can be used to test predictions from mantle circulation modelling. Some of these constraints relate to present-day observations (seismic, surface deflection) and the others to observations over time. Equally, some of the observations are sensitive to properties near the surface (e.g. surface deflection and melting) and others the whole mantle volume. This combination of disparate observations will provide tighter constraints on mantle circulation than any single observation alone.

We remind the reader that when undertaking the comparison one needs to consider the limitations of the MCM and/or observations—for example we can expect that a detailed crust and lithosphere structure is probably required for a good comparison with surface deflection. We note that we have only presented a subset of possible observations that could be used, many others are mentioned in other contributions to this issue. We have also not discussed the possibility of using variational data assimilation with MCMs using adjoint methods (e.g [157,158]), a powerful extension. Another contribution in this issue will illustrate the power of applying multiple observational constraints simultaneously to a number of models.

The MCM presented here fits some observations reasonably well (long-wavelength lower mantle seismic structure, splitting of normal modes, shallow seismic structure of Pacific basin, spread of temperatures at MOR, differing amount of depletion between OIB and MORB source regions) and others less well (e.g. paleomagnetism, surface deflection, subduction zone seismic structure, upper mantle seismic anisotropy and U isotopes). This varying misfit suggests that applying such a disparate group of observations will allow much to be learnt about mantle circulation.

Data accessibility. Simulation data and unpublished code used in this work are available at [159].

The data are provided in electronic supplementary material [160].

Declaration of AI use. We have not used AI-assisted technologies in creating this article.

Authors' contributions. J.H.D.: conceptualization, funding acquisition, methodology, project administration, resources, software, supervision, validation, visualization, writing—original draft, writing—review and editing; J.P.: data curation, formal analysis, investigation, methodology, software, validation, visualization, writing—original draft, writing—review and editing; I.A.: formal analysis, investigation, methodology, software, visualization; M.A.: funding acquisition, methodology, supervision, writing—review and editing; P.B.: formal analysis, investigation, methodology, software, writing—original draft, writing—review and editing; A.B.: conceptualization, funding acquisition, methodology, supervision, writing—original draft, writing—review and editing; C.D.: conceptualization, funding acquisition, methodology, software, writing—original draft, writing—review and editing; T.E.: conceptualization, methodology, supervision, writing—review and editing; Y.A.E.: formal analysis, investigation, methodology; V.M.F.: formal analysis, investigation, methodology; A.M.G.F.: conceptualization, funding acquisition, supervision, writing—original draft, writing—review and editing; S.F.: writing—original draft; S.G.: software; B.J.H.: writing—review and editing; P.K.: conceptualization, formal analysis, funding acquisition, methodology, software, supervision, visualization, writing—original draft, writing—review and editing; F.L.: formal analysis, investigation, methodology, software, visualization, writing—original draft, writing—review and editing; W.L.: data curation, formal analysis, methodology, writing—original draft, writing—review and editing; G.J.M.: methodology, writing—review and editing; S.M.: formal analysis, investigation, methodology, writing—original draft, writing—review and editing; R.M.: conceptualization, formal analysis, funding acquisition, investigation, methodology, supervision, writing—original draft, writing—review and editing; A.N.: conceptualization, funding acquisition, methodology, software, supervision, validation, visualization, writing—review and editing; C.P.O.: data curation, formal analysis, investigation, methodology, software, writing—original draft; A.P.: writing—review and editing; D.P.: conceptualization, funding acquisition, supervision; N.R.: writing—review and editing; G.G.R.: conceptualization, formal analysis, funding acquisition, investigation, methodology, software, supervision, writing—original draft, writing—review and editing; J.B.R.: formal analysis, investigation, methodology, visualization, writing—original draft, writing—review and editing; J.S.: data curation, methodology, writing—original draft, writing—review and

editing; O.S.: conceptualization, funding acquisition, investigation, methodology, supervision, visualization, writing—original draft, writing—review and editing; W.S.: formal analysis, investigation, methodology, software, visualization, writing—original draft, writing—review and editing; A.M.W.: conceptualization, formal analysis, funding acquisition, investigation, methodology, software, writing—original draft, writing—review and editing; J.Wa.: formal analysis, investigation, methodology, software, writing—original draft; J.Wo.: conceptualization, formal analysis, funding acquisition, methodology, software, supervision, validation, visualization, writing—original draft, writing—review and editing.

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