

RC2:

The manuscript presents a geodynamic study that investigate the use of configurational entropy to characterise the mixing property of a model, and comparing a variety of models. One expressed goal is to use this measure to understand some geophysical and geochemical observations. Maybe it is because it is a paper about mixing, but I have a mixed analysis of the work. What I appreciate the most is the quality of the geodynamics models, of the data analysis and how the results are presented. It is impressive to have that in a paper, and it provides a lot of confidence in the outcomes. The shortcomings to me come from the target of the study, which is not yet found. My feeling is that it comes from the lack of inclusion of the literature about mantle mixing (maybe because most of it was published before 2010), and the duration of the simulation being 1 Gy that is too short to discuss primordial heterogeneities.

We appreciate the praise by the reviewer on how our manuscript is written. We agree that the manuscript is lacking mixing literature and accordingly added a summary of published mixing-studies using other quantifications in the introduction. We do not compare our results to geophysical or geochemical observations and we merely discuss how this entropy may be useful to compare model results with those observations. Therefore, we also changed the wording of 'primordial' to 'original' when presenting our results and only use it when discussing potential applications or other literature.

*Excerpt 1: "While mixing technically involves diffusion at small scales and the term stirring has been proposed to account for the mechanical stretching and folding (Farnetani & Samuel, 2003), which is infact our interest here, we shall nevertheless use the term mixing in the remainder of the manuscript as we use varying 'compositions' that are able to mix.*

*It has long been recognized that mantle convection is complex, and its mixing has been studied for decades, see (Kellogg, 1993; van Keken et al., 2003) for early reviews on this topic. Unsurprisingly, the advent of high-performance numerical modelling in the mid-90's saw a resurgence in the characterization of mantle mixing and its quantification. Various approaches have been proposed over the years, but the vast majority of these are based on the time evolution of a swarm of particles. Early studies (such as (Hoffman & McKenzie, 1985; Olson et al., 1984a, 1984b; Richter et al., 1982; Schmalzl et al., 1996)) use statistics to arrive at a mixing time scale. Another approach using the presence, addition, and/or removal of particles in a modelled domain is used to quantify mixing-times and degassing (sampling of primitive mantle) (Gottschaldt et al., 2006; Gurnis & Davies, 1986a, 1986b), to measure strain and the dispersal of tracers (Christensen, 1989; Kellogg & Turcotte, 1990) or to study the development of time-dependent mantle-heterogeneities (Hunt & Kellogg, 2001). Note that other methods have been proposed, such as a line method (Ten et al., 1998), a correlation dimension method (Stegman et al., 2002) and a hyperbolic persistence time method (Farnetani & Samuel, 2003).*

*More recently another approach has dominated the mantle mixing literature: it consists in measuring the Lyapunov time, which is the characteristic timescale for which a dynamical system is chaotic, or rather its inverse the Lyapunov exponent. It can be shown that mixing is laminar or turbulent by evaluating the Lyapunov exponent, the larger the exponent the more efficient the mixing is. A typical example uses a steady state velocity pattern obtained in a 3D spherical domain to advect passive particles (van Keken & Zhong, 1999). They use a very common approximation to the Lyapunov exponent, i.e., the Finite Time Lyapunov Exponent, which is based on the evaluation of the distance between a multitude of particle pairs that are initially very close to each other (i.e., stretching of this original distance after 4 Ga). This shows a strong diversity in mixing behavior dependent on the mantle flow characteristics. Other studies that used the same approach in studying a variety of mantle convection problems include: (Bello et al., 2014; Bocher et al., 2016; Colli et al., 2015; Coltice,*

2005; Coltice & Schmalzl, 2006; Farnetani et al., 2002; Farnetani & Samuel, 2003; Ferrachat & Ricard, 1998, 2001; Samuel et al., 2011; Tackley & Xie, 2002; Thomas et al., 2024).”

The first studies of mantle mixing date back to the 1980's and one of the difficulty was to deal with scales. So 2 approaches were taken: one dealing explicitly with scales, such as the authors do here with configurational entropy. It was in relationship with the observations of heterogeneities at all scales (marble cake like at first, more comprehensive nowadays with mid-ocean ridge heterogeneities etc...). The other approach is to work with the theory of dynamic systems, because mantle convection is chaotic. The use of Lyapunov exponent characterize the local and global properties of stretching of heterogeneities. Mixing happens when an heterogeneity is stretched at a scale at which chemical diffusion operates. This scale for the Earth is about 1cm I would say (some papers talk about it). Lyapunov exponent are a form of stretching rate when mixing is chaotic. I think Ferrachat and Ricard introduced it in 1998. Configurational entropy and Lyapunov exponent can be related with Ergodicity theory. It is fundamental to acknowledge the literature more extensively here and situate the innovation of the study. As the authors say, Naliboff and Kellogg in 2007 already used this measure, so the paper cannot really be the introduction of this measure. It has to be more than this (which I think it can be, but more explicitly). And it is also important to relate this measure to the Lyapunov exponent studies. At the end of the day, the stretching rate scales with the velocity in mantle convection. So faster velocities imply better mixing, which is what is observed here in the models as well.

We thank the reviewer for his comments regarding mixing studies from the 90's. Therefore, we have taken these suggestions above and the suggested authors at the end of the review and incorporated them in our manuscript. See the excerpt from the introduction in the manuscript above. We think that a full comparison between the Lyapunov exponent (or time) and the global entropy goes beyond the scope of this work as the global entropy also depends on the varying compositions in a model rather than just the mechanical stretching. We added a section to the discussion explain this point of view, see below. We must admit that we do not fully understand the Ergodicity theory and therefore refrain from mentioning this term. We have focussed the manuscript more on the additional variable of composition (which was not in Naliboff and Kellogg 2007) rather than just stretching of the entire domain.

*Excerpt 2: “A direct comparison between configurational entropy and other measures used to quantify mixing, like the Lyapunov exponents (or time), is beyond the scope of this work. We see two arguments in favor of configurational entropy for specific uses: 1) its measurement does not require an integration over time thereby providing instant values for local and global entropy and 2) its flexibility, since the spatial distribution of any field carried by the particles, passive or active, such as chemical composition, water-content, reached depth or temperature, can be quantified.”*

*Excerpt 3: “In such models the Lyapunov time would be useful to quantify the deformation, or stretching, in the mantle (e.g., van Keken & Zhong, 1999; Coltice 2005) or quantifying uncertainties in twin-experiments (e.g., Bello et al., 2014; Bocher et al., 2016).”*

There is an issue I think with the duration of the simulation. They are 1Gy long. It seems long, but it is not for a mixing study because (1) radiogenic geochemical heterogeneities needs time to develop and they mostly show preservation of >2Gy, (2) 1Gy is a little more than one mantle overturn today if we consider a slab takes 200 My to reach the bottom of

the mantle, (3) primordial mantle means it is almost as old as the Earth and (4) mixing/erasing heterogeneities at melting regions rates in the ancient Earth seemed much faster than today.

We agree that primordial is not right term to use in our model spanning 1 Ga, therefore we have changed it to 'original lower mantle material' when presenting our results. To use the term primordial one should indeed run models longer (e.g. 4 Ga) but also incorporate the mixing and evolution of mantle composition and the varying styles of convection and tectonics for example caused by higher temperatures than in today's mantle.

For the geodynamic community, 1Gy of preservation at the slow mantle convection rate of today is no surprise and does not necessarily teaches us about preservation of primordial heterogeneities. When working with Lyapunov exponent, it is important to run the simulation for a time sufficient to obtain finite time Lyapunov exponent. I am not sure 1 Gy would be sufficient here. So in this study, the setup and the methods are great, as good as they can be, but my appreciation is that the target of the study is not completely mature. I suggest refining the research objective, as aligning the study with previous work and integrating observations could significantly enhance its relevance.

We have focussed our contribution to stress the relevance of using varying compositions when using the entropy calculations, as it can also be used in regional models with mixing on shorter timescales, see excerpt 2.

Ultimately, this approach could elevate the study, making it a substantial contribution to the field. A minor detail: in cylindrical geometry the volume of the lower mantle is larger than in spherical geometry. To compare with Earth, maybe the geometry regions that mix in the study could be scaled by volume instead of depth? For the literature, I suggest to integrate papers by D. Turcotte, with L. Kellogg, also works of M. Gurnis and G. Davies, works of S. Ferrachat, Y. Ricard, of H. Samuel, of U. Christensen, P. Olson, P. Van Keken.

We have integrated the works of the suggested authors in the introduction and thank the reviewer once again for pointing those to us. We also added a remark regarding the cylindrical/spherical scaling in our set-up, for instance regarding equal volume cells when applied to 3D models.