

Thank you very much for your insightful review. We have included your comments below in **black**, and our responses are written in **blue**.

Abstract. L.2: Do you mean phase transitions in the strict sense or also mineral reactions in general. It is common in the geoscience community to confuse mineral reactions to phase transitions s.s. – especially for a system with many components that involves solid solutions.

Thank you for your comment. We agree that different geoscience communities have different working definitions of the word “phase transition”. We have decided to adopt the common geodynamic meaning of phase transitions, which corresponds to all mineral reactions that take place over a limited P-T range and have a noticeable effect on material properties. We have defined this in the introduction, and have also made explicit that the mineral physics community has a different definition.

L6: Your previous work did not **formulate** the energy equation in terms of entropy – this is a textbook result. Your work **used** the entropy formulation (which admittedly has advantages to the classic temperature forms under certain conditions).

Thank you for pointing this out, you are correct. We have gone through the text to improve this wording, and now also cite classic textbooks such as Schubert et al., 2001 (also cited in our previous work), and some older literature such as de Groot and Mazur (1962) when mentioning the formulation.

L.9: Although your method shows potential and has advantages, it is not thermodynamically consistent in the strict sense of the term. My reasoning is as follows: the projected density approximation is still an approximation compared to the true density (as you have in equations 1-3). I am aware of your previous work and arguments (following Gassmoller et. al. 2020) against using the true density and pressure oscillations. The arguments used there are related to computational limitations rather than physics. This is not mentioned as a criticism to the authors for their numerical schemes or abilities – “soundproofing” of numerical, compressible codes has been a problem in many communities (i.e. atmospheric models). Therefore, I agree that this is a good approximation but calling it just “fully consistent” is a bit misleading. More consistent to previous attempts yes, “fully consistent” I would disagree.

We agree, and we have removed the word ‘consistent’. We now also note in Section 2.1 where we discuss the equations, that we neglect the effect of dynamic pressure on the thermodynamic state (at the end of the second paragraph).

L:20: citations to early works that brought attention to this matter in the framework of convection simulations would be needed here (e.g. Schubert & Turcotte, 1971 – Schubert et al. 1975 and goes on).

Thank you for this suggestion. We now cite more early works, including these two suggestions.

L:25: As before, the role of phase transitions was known before Faccenda and Dal Zilio, (2017). Please use “e.g.” or cite relevant earlier papers.

We have changed it to “see review by Faccenda and Dal Zilio, 2017, and references therein.”

L:39 (citation to Billen, 2008) – As before. I understand that the authors need to cite something, but all these are general statements that are known for decades, please use “e.g.”. Otherwise, the reader who is not familiar to this literature may think that all these phenomena became known after the 2000s... I will stop making comments of the same kind because this is not my role to add references. However, I encourage the authors to give more credit to original literature (when general statements are made) or use “e.g.” to emphasize that these are examples. For example, all the work in compressible convection from Trubitsyn and co-workers, Ricard and co-workers has been ignored.

We now use “e.g.” here and in many other places throughout the manuscript. In the revised manuscript, we cite the work of Trubitsyn and Ricard in Section 2.1, where we discuss our approach to modeling compressibility. We also cite de Groot and Mazur (1962) in the discussion of the entropy equations, and de Groot and Mazur (1962) together with Ricard (2015) in the discussion of solving the mass conservation equations for each bulk composition.

L:62: Simplified expressions are not necessarily bad. In fact, simple systems will have sharper phase transitions and “jumps” compared to more complex chemical systems. Thus, in such cases the hydrodynamic instabilities may be even more severe and produce more complex results in the hydrodynamic sense. Thus, it is not a matter of complexity, it’s the fact that you aim to be more realistic.

We agree, and we have changed the text to now say “Although they can capture the thermodynamic behavior of individual phase transitions, such parametrizations are unable to capture the full complexity of reactions in the mantle”.

L:69: By the use of the word “transitions” in this sentence you mean mineral reactions in general. Please be specific to thermodynamic terminology.

Thank you for your comment. We agree that we are not abiding strictly by thermodynamic terminology, but are rather adopting the common geodynamic terminology. We have made this clear in the introduction.

L:71: Please add a reference to that statement. Which kind of solution you are referring to? There are numerous works on the Stefan problem that solve such things.

Thank you for pointing this out. Our statement refers specifically to the formulation commonly used in geodynamic simulations, where latent heat effects are incorporated through thermodynamic derivatives (effective thermal expansivity and specific heat). At univariant phase transitions, these derivatives make this particular formulation mathematically ill-posed. We have rewritten the text accordingly and now point the reader to section 2.3 in Dannberg et al., 2022 for more detail.

L:74: You didn't introduce the entropy method; you used it and implemented it in this community. This formulation is known in textbooks.

Thank you for pointing this out. We agree that the fundamental entropy formulation has been established in the classical thermodynamics literature and was not introduced by our previous work. Our original intention was only to introduce this numerical implementation as a method to model sharp phase transitions. We have now revised the text to clarify that the formulation is not ours and added citations to the classical thermodynamics literature.

L:103: Please add a reference on how the effective properties are obtained.

We calculate the effective properties based on the thermodynamic database from Stixrude and Lithgow-Bertelloni (2022). We have added the reference.

L:117: This is the heart of my criticism regarding thermodynamic consistency. The use of a hydrostatic pressure instead of the true pressure is a gross simplification that neglects important physics such as the ΔV of reactions (and phase transitions) as a response to dynamic pressure variations. I understand why you do it and I do not object to that, but please change the wording the statements regarding "consistency" and accuracy. It is a better (or improved) approximation compared to what you had before.

We have removed 'consistent' and also noted that we neglect the effect of dynamic pressure on thermodynamic states

L: 144-150: Your assumptions on the reactivity are a bit difficult to justify in general (or I am missing something here). How would you reconcile the case where the modal amounts of minerals change during P-T changes?

We think that there is a misunderstanding here that arises from our use of the word "component" in ASPECT, which differs somewhat from the common thermodynamic definition. Within a single ASPECT-component ("bulk composition"), modal amounts (and compositions) of minerals are allowed to change during P-T changes—these changes are captured implicitly by the lookup table. What is not allowed in our scheme is chemical exchange *between* ASPECT-components, which correspond to (for example) a chemically equilibrated peridotite or basalt of fixed bulk composition.

To avoid confusion, we now use composition or bulk composition instead of "component".

Eq. 9: If I understand correctly by "component" you mean mineral phases as mechanical mixtures. Correct? If yes, please state it – I had to go at the end of the manuscript to understand it. If not, please specify what you mean by "component" (i.e. chemical component)? If it is a chemical component, then your advection equation needs further justification (i.e. negligible diffusivity across phases etc).

The “component” in our original text refers to an “equilibrated material of fixed bulk composition”. We have now changed the wording to “bulk composition”, and given more detail when the term first appears (line #141 in the revised manuscript).

We now also specify the assumptions that go into our conservation equations for the chemical compositions (see also answer below).

L: 209: “Smoothing” the thermodynamic lookup tables is not always a consistent approach. It depends on resolution and on the accuracy of capturing the “step” in case of phase transitions. For example, in your figure 8 (left side) it is actually very poorly resolved at the boundaries around 24 and 10 GPa (i.e. it is not sure if you “hit” the transition or if your material goes through the “pixels” that indicate the transition).

Our original Figure 8 (now Figure 9) shows the thermal expansivity in pressure–temperature–space (rather than pressure–entropy–space), because these are the variables that most geodynamicists will be used to. Some phase transitions are very thin and are not captured well in P-T space. This is the problem that our approach fixes: (a) the phase transition is broader in entropy space (see Figure 2 from Dannberg et al. 2022 posted in our reply to Reviewer 1 above), and (b) we do not need to accurately “hit” the transition in our table, because we do not use the thermal expansivity in our equations.

With reference to smoothing our thermodynamic tables (Section 3.3), we note that while this is not always an *accurate* approach from the perspective of phase relations, it is a *thermodynamically consistent* approach (the relationships between thermodynamic derivatives properties, and Maxwell’s relations are all preserved by the smoothing). There are a few reasons for smoothing the enthalpy in entropy–pressure space; these are summarised in our response to Reviewer 1’s comment on Figure 2.

L:297: In the problem of mass conservation, I noticed that your advection equation of the “component” lacks density and it is given in the non-conservative form. Thus, your “component” approach is prone to problems with mass conservation, how do you monitor it?

We use the form of the mass conservation equation for chemical compositions commonly used in geodynamic applications (for example, given in Ricard et al., 2015, Treatise on Geophysics: Physics of Mantle Convection, Equation 158, and also in de Groot and Mazur, 1962). Our X_i are the mass fractions of our chemical (bulk) compositions, and we assume the Eulerian form of the equations, neglecting diffusion and reactions between chemical compositions. This means we can divide Equation 158 by the bulk density. The velocity $\mathbf{u}$ is the velocity of the center of mass.

We have revised the text and added the references given above.