Dear editor,

At first, we would like to thank the reviewers for taking the time to read and provide comments on our work. Although critical, the reviews allowed us to further develop our arguments and expand points that needed further explanation. In brief, we have modified the text summarizing the assumptions for our specific diffusion equation and highlighting that the full derivation is available within the Appendices as required by reviewer 1. Following the comments of reviewer 1, we have written Appendix C, and we have updated the figures 2, 3 and 12 (old numbering). In addition, and in response to the comments made by reviewer 2, in the new version we have implemented an additional refinement method (h-refinement). This allows the users to choose what kind of refinement method they want. For this reason, the respective part was expanded and the text was modified. Regarding other minor/moderate points, please find our detailed answers below.

On behalf of the co-authors,
Annalena Stroh

Reviewer comments are written in black whereas our answers are given in blue.

Reviewer #1 (Pierre Lanari)

To improve the clarity of the text for a more general audience (e.g. potential users), the following suggestions could be implemented:

In geology, cation diffusion in minerals is often modelled using mass or mol fractions. However, if I am not mistaken, equation 1 is correct for concentrations, which are mass/volume or mol/volume. It is possible to use equation 1 with mass or mol fractions, assuming that the density of the mineral remains constant (which is unlikely to be the case for major elements in a single crystal, and even less so between a crystal and a melt, or an intergranular medium with aqueous fluids). This is something that needs to be clarified. In the current manuscript, the terms 'compositions' and 'concentrations' are used rather loosely, so it would be great if these were clarified at the beginning of the text. A concentration is always a quantity for a given volume. It is only in equation 19 that it becomes clear how the two cases are handled. This is something that is not always used correctly in the literature, and this work would benefit from clearly explaining the correct way to do it to potential users.

We thank the reviewer for this comment, and we agree. In fact, Appendix A has been written to explain the differences and provide a detailed derivation of how 'compositions' and 'concentrations' are related in our manuscript (together with the simplifying assumptions used). However, we note that putting all this important information at the end may lead to confusion. For

this reason, we have homogenized the terms using "composition" as the primary function in the main text. To emphasize these points, we have now modified the text before the introduction of Eq. 1 in order to avoid confusion.

The title of the paper refers to 'geospeedometry applications'. Are there any plans to add inversion functions that would allow users to perform geospeedometry? Currently, the package appears capable of simulating diffusion in complex cases, but it is not yet ready for working with natural data and for example obtaining T-t trajectories. If the growing/resorption rate is unknown, a moving boundary model will seriously limit the possible applications of geospeedometry. I could be wrong, but including an example of a geospeedometry application using natural data would be beneficial for the readers. Alternatively, perhaps this term should be removed from the title.

We thank the reviewer for this comment. While writing this manuscript, our intention was to emphasize on the benchmark cases and test for accuracy for all the various cases that were treated. In fact, adding the examples (B1, B2), chapter 3.2 was prepared to show the applicability of our package in geospeedometry applications. In the original paper of geospeedometry (Lasaga, 1983; cited in the main text), a very similar (and mathematically identical) time-transformation technique was used as our forms in Eqs. (23, 24) and we have used the results of the transformation to benchmark the accuracy of our time integration. The combination of K_D, and D that change in time with accurate time integration allows the usage of our approach for geospeedometry applications. We understand that our initial manuscript did not emphasize the previous point sufficiently. For this reason, we have now modified "Discussion and Conclusions" to emphasize the potential geospeedometry applications.
Finally, we would like to note that the classic geospeedometry applications did not consider the moving boundary problem. As the reviewer correctly pointed out, the consideration of moving boundaries may require knowledge of the reaction progress (examples in chapters 3.3 and 3.4), for such cases, our approach can be used to place constraints on the reaction kinetics via the forward modelling of crystal overgrowths or resorption zones. We have modified the "Discussion and Conclusions" part to emphasize this possibility.

Specific comments

Lines 8-9. What is high temperature? This can be observed in hydrothermal systems, but these are not high temperature.
In relation to solid-state diffusion, high temperature is always related to the homologous temperature and the nature of the material. However, since this part is in the abstract, we do not want to be too specific. Instead, we have modified the text to refer to "relatively high temperature" (since different minerals have different melting temperatures).

Line 15. Before you talked about concentration. Is there a reason to switch to concentration that is quantity/volume.

In our models, when we consider a given phase (intra-phase diffusion), the distinction of concentration and composition gradients is relevant only when significant gradients in density are present. We have provided more details in appendix A to clarify these points. However, we understand the point of the reviewer that switching terms may cause confusion. For this reason, we use "composition(al)" throughout for clarity and we refer to concentration only when it is necessary.

Lines 18-19. Be careful that we usually don't have/use concentration data (mass/volume).
As for the previous comment, we have changed the terms throughout for clarity.

Lines 66- 69. In Fick's second law isn't that a concentration (e.g. mass/volume)?
The reviewer is correct in his assumption regarding the original version of Fick's 2. law. However, compositions can as well be used (compare Appendix A). We have modified the text to clarify these points.

Line 70. Is that assumption valid for a crystal and an intergranular medium?
It is mentioned that Eq. 1 is valid for the diffusion within a particular phase. We have now modified the text and added "(intra-phase)" diffusion in brackets to avoid confusion.

Line 72. Diffusivity, right? -> always depends on composition
Yes, this was a typo and we have corrected, it was diffusivity.

Lines 97-100. This is unclear to me.
In the new version, we use composition throughout. Therefore, the text is now corrected.

Lines 110-111. I think that those are not variables and therefore should not be in italics.
We have modified the text according to the reviewer's suggestion.

Lines168-169. Something I don't fully understand here is that the reaction velocity in general depends from an activation energy and ΔG terms, here it seems to be poorly controlled by the flux. It would be interesting to clarify to what cases this equation applies. – It wound't apply for examples to polymorphic reactions where the concentration gradient is zero.
As far as compositional gradients are modelled, Eq. (18) can be used in the diffusion-controlled growth (or resorption) regime. We note that near the equilibrium limit an overstepping in composition results to an overstepping in Gibbs energy. This overstepping is why the approach that we use is widely used in metallurgy (see Balluffi et al., 2005 – cited in the main text). We have now modified the text for clarity.
Regarding the cases of pure phases (not considered in our manuscript) the original form of Eq. (18) was discovered for the case of ice melting (the classic Stefan problem) but using energy (heat) and not compositional gradients. Therefore, we find that this approach is well justified if used in the diffusion limited regime. The interested reader can find many examples in the book of

Rubinsteĭn (cited in the main text) that span from pure phases (like the classic Stefan problem) to solution models (as in our case).

Lines 179-184. Abbreviations should not be in italic, only variables.
- As well Linies 204-205, Table 3, line 308

We agree with the reviewer, and we have modified the text accordingly.

Lines 207-208. This is clear and correct! It would be good to be clear before in the manuscript!

We thank the reviewer for this comment and agree. We rewrote the parts before to clarify the used assumptions.

Fig. 2. Current: What do you mean by "current"?
- As well Fig. 3

We meant the numerical calculated composition at the end of the simulation. We have now changed the legend accordingly.

Table 3. Composition: Unclear? In Fig. 4 concentration is used.

We have adjusted the use of concentration and composition and checked all figures, tables and captions again to ensure they are used correctly. K_D and M_R define variable names. We prefer to leave D and R in italic.

Lines 352-355. Maybe the figure could go in supplementary material and you could simply mention that it closely resembles

We have created Appendix C (following the GMD guideline for supplementary material) and implement the reviewer's suggestions.

Lines 368-369. Now it is clear, it wasn't before!

We thank the reviewer for the helpful comment and mention the use of arbitrary reaction rates earlier in the manuscript.

Lines 385-387. Again, this could go to supplementary material without affecting the manuscript.

We thank the reviewer for recommending and moved this part to Appendix C.

Line 416. Not Italic.
- As well Line 430

We thank the reviewer for spotting this error. It is fixed.

Fig. 12. X_{Fe} not italic; T, t italic

We thank the reviewer for his comment and changed the figure.

Lines 521-529. I would recommend adding part of this to the main manuscript.

We have changed the text according to the reviewer's suggestion.

Reviewer #2 (Lyudmila Khakimova)

The manuscript presents a new numerical framework aimed at simulating 1D diffusion, moving-boundary problems, and coupled diffusion–growth processes in mineral systems. This class of problems is central to geospeedometry and diffusion chronometry, where an accurate treatment of compositional discontinuities at mineral interfaces and time-dependent boundary conditions is essential. The paper is clearly organized and methodologically transparent, offering extensive benchmark comparisons against analytical solutions. The numerical formulation (Galerkin FEM, adaptive mesh, regridding and PCHIP interpolation) is described in sufficient detail for reproducibility. The examples convincingly demonstrate that the approach is robust and flexible, and the open-source implementation in Julia is a strong asset for the research community.

We thank the reviewer for the constructive criticism, and we have already implemented h-refinement as an additional option on the side of the user. We believe that this option makes the paper stronger and allows more flexibility in future development. Please find our response to the specific points below.

I have only a few suggestions that may further strengthen the manuscript.

The geometric-progression–based interface refinement is elegant; however, a brief comparison with more conventional h-refinement criteria (e.g., gradient-based error indicators commonly used in FEM) could help readers understand why the chosen approach is particularly advantageous for resolving sharp compositional discontinuities.

As previously mentioned, we have now implemented the h-refinement approach as it is commonly done in FEM analysis. We have also expanded the text accordingly. However, we have chosen not to implement an error-driven refinement approach (i.e. the level of refinement would be given by an error estimator) since this would result to the change of the number of elements according to the magnitude of gradients/errors. We would like to avoid this approach since it would make the code much slower due to the many allocations needed. For that reason, we have implemented two strategies for h-refinement (explained also in the text). In the first strategy the user can specifically choose the refinement levels whereas in the second strategy the user choses the length ratio between the largest and the smallest element. Both approaches lead to a fixed number of elements/nodes during the simulation that offers a computational advantage.

Please see below two cases, one continuous (B1), and one discontinuous (B5) that were calculated with our h-refinement approach. The results show that the solutions can be also reproduced in that case.
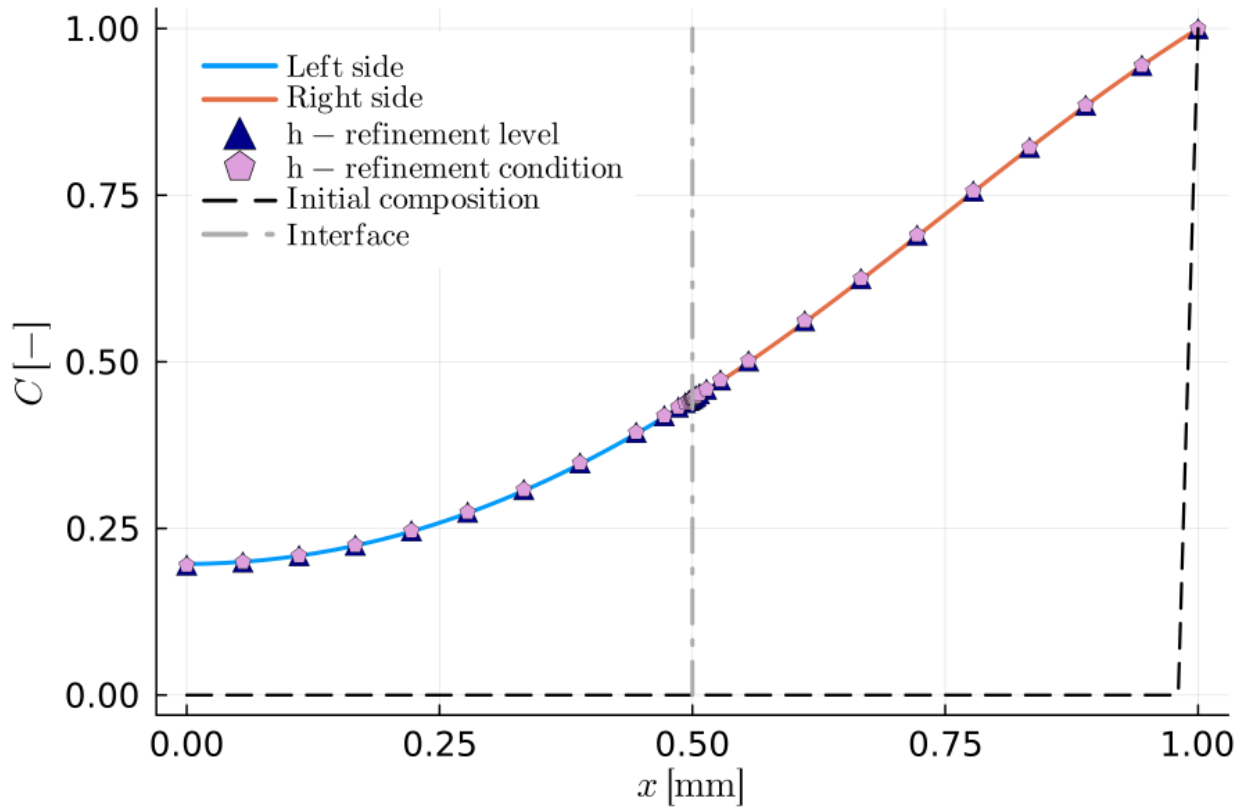
Example B1 solved for the case of the two h-refinement approaches (see main text for more details). In the "h-refinement level" solution we performed the refinement by choosing a fixed number of refinement levels. In the "h-refinement condition" we performed the refinement until the length ratio of the largest to the smaller element is the same as the one that was chosen by the user. The solid lines indicate our original refinement approach (m-refinement).
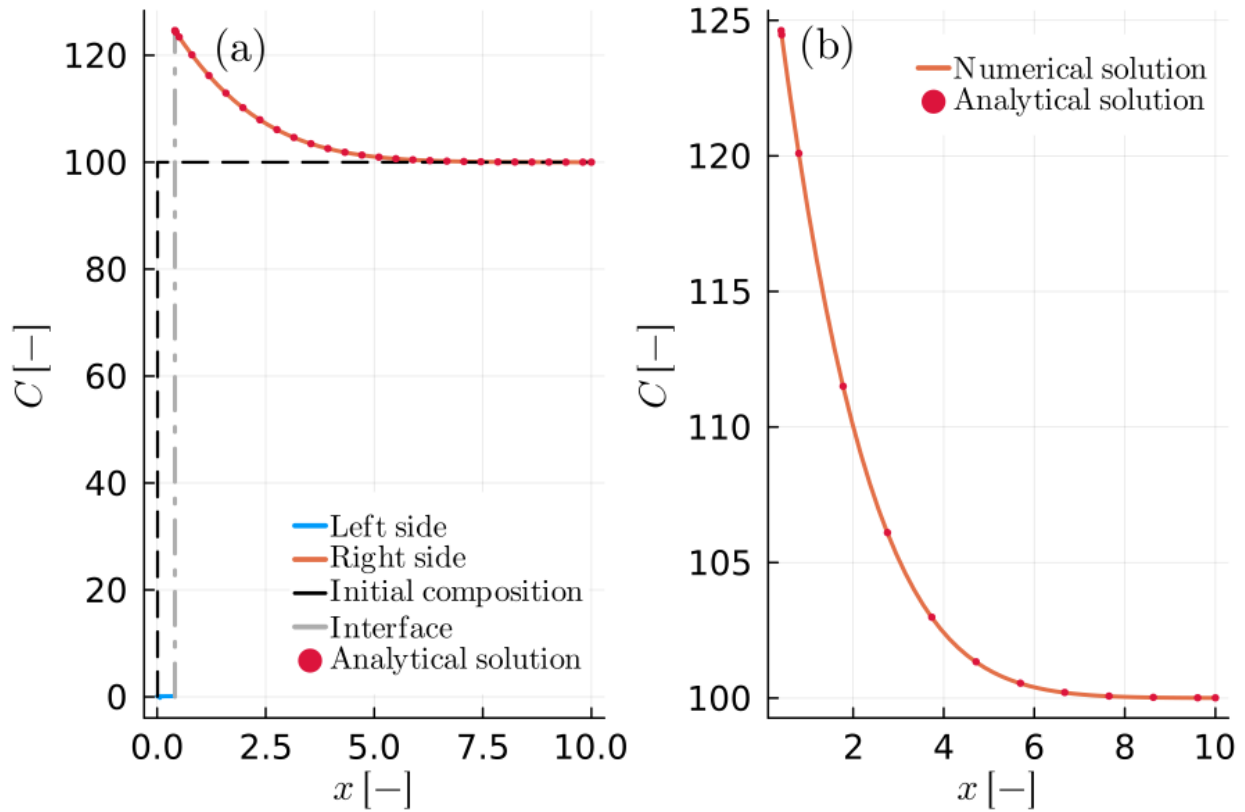
Same calculation as for example B5 (Fig. 7 in the new version of the manuscript). This example was calculated with the h-refinement approach using initially 50 nodes and 3 refinement levels.

Our previous results show that we can obtain the same solutions as in the original approach.

It would be interesting to comment on how well the adaptive grid and interpolation strategy can resolve extremely steep concentration gradients at mineral interfaces. Are there specific requirements or constraints on the numerical scheme to ensure conservation and consistency when gradients approach discontinuous behavior?

We have not investigated in detail the performance of the adaptivity. It should be noted that the optimal refinement depends on the particular problem that is under investigation. For example, in case of no-growth where the size of the crystals remains the same and the gradients are concentrated at the interphase boundary, the h-refinement will be the optimal choice (since it targets the gradient specifically). In more general cases though, the m-refinement approach offers a compromise on the resolution of compositional profiles.

These are minor points, and I offer them in the spirit of further enhancing an already strong manuscript.

We thank the reviewer and we really appreciate the opportunity to enhance the code and the manuscript.

In conclusion, I would like to sincerely thank the authors for this carefully executed and clearly presented study. I truly enjoyed reading the manuscript and appreciate the effort that went into developing this contribution.

Finally, we would like to thank both reviewers. Their points were considered and we hope that the editor will find our changes appropriate.

On behalf of the co-authors,
Annalena Stroh