

I find the manuscript entitled “Modelling chemical advection during magma ascent” by Dominguez et al. quite interesting and helpful for the geoscience community. In my view, the problem of numerical advection is often underappreciated, and the presented study clearly shows the pitfalls of using too simplistic advection schemes. In their work, the authors introduce and compare the performance of four selected numerical advection schemes. In conclusion, they advocate the usage of the WENO type of schemes for petrological applications (chemical advection). Below I give my general and detailed suggestions that the authors may consider to follow before the final publication of the manuscript.

The numerical schemes selected for the study are introduced as simplified 1D variants and later tested using 2D setups. Although the 2D generalizations are rather straight-forward, in my view, it would be worth to give some clues to the readers on how they are developed. In particular, the 2D generalization of the WENO scheme that builds on a 5-point stencil in 1D is perhaps least obvious in this respect (not to mention the treatment of the boundary conditions). In fact, in the final parts of the manuscript, the authors themselves mention an alternative formulation for the 2D WENO scheme that builds on a 3x3 stencil.

Response: The extension of the WENO scheme to 2D is rather similar to the extension of an upwind scheme to 2D, where each flux term for each dimension is simply calculated independently and summed up at the end before the time stepping procedure, so that each dimension can be treated independently as described in 1D.

→ Explanations have been added in the revised manuscript.

The mention of the compact WENO was mentioned to give an alternative to readers who are not interested in using parallelizable code for less computationally expensive applications, as it reduces to the use of one ghost point for the boundaries. Also, the mention of the compact WENO reconstruction is not something specific to 2D or 3D but is also applicable to 1D. It is simply an alternative discretization that uses an implicit stencil, hence allowing smaller stencils. The cost is that this requires to solve a linear system at each timestep, which is not easily parallelizable. Both reviewers showed that this was confusing, so the mention of the compact WENO scheme has been removed from the manuscript.

→ The notion of compact WENO has been removed from the conclusion.

I was a bit confused about the MIC scheme that was used in the study. The authors mention the initial step of interpolating the field values from grid nodes to markers. Considerable focus was given to integrating the trajectories of the markers. The step of interpolating the field values back from markers to nodes was sketched out. Unless I got it wrong, the advected fields in this study are essentially phase fields, so no calculations and updates need to be performed on the Eulerian grid. Thus, there is no need to interpolate back these updates to markers in such cases. However, interpolating the base field values from grid nodes to markers would be an undesired and suboptimal step leading to unnecessary numerical diffusion. I think that it would be helpful to clarify the design of the MIC scheme that was used in the tests. What is the reason for the observed mass loss in the second test using the MIC scheme? Could it be related to the non-conservative reseeding and removal of the markers? I would suspect that the mass conservation of the standard MIC should be almost ideal.

Response: in the tests, there is indeed no need to reinterpolate between the markers and the grid as a passive advection is performed. Nevertheless, the focus of this paper is to find the best

solution for advecting the chemical composition of a melt, with the ultimate goal of moving towards reactive transport modelling, as it is mentioned in the introduction of this paper. With this in mind, the authors believe that it is relevant to include a reinterpolation step, since in fully coupled system, the change in viscosity and density of the melt induced by the change in chemical composition will have an important effect on the two-phase flow. As this step is not required in the other numerical schemes as they are performed at the grid points, the authors believe that it is relevant to add this step for a fairer comparison between the different advection schemes.

→ This was mentioned in the manuscript.

Concerning the mass loss observed in the MIC scheme for the coupling with the two-phase flow, there was a mistake in the implementation of the scheme (as well as for the QMSL). The results after correction show way less mass loss, probably reflecting more what the reviewer has in mind. This mass loss can be indeed attributed to non-conservative reseeding and removal of the markers.

→ New results after correction of the MIC implemented were added to the manuscript

The author presented the rigid-body rotation test as their base test. In my view, a bit more complex synthetic 2D test such as for example the shear cell test would be a great addition to the study. On a different note, I actually wonder how to design a balanced comparison of the accuracy of grid-based advection schemes against marker-based methods, when their numerical resolutions largely differ (for a fixed grid resolution, a much larger number of markers is used than nodes in this study). In addition, the authors took advantage of the extended stability of the MIC and SL schemes and used a larger value of the time step than in the case of the upwind and WENO schemes, however, this may have an effect on the numerical performance of the studied schemes.

Response:

→ A new 2D test was added in the revised manuscript, a convection test using a parametrised equation for the velocity field simulating the advection in a single convection cell.

The question on how to properly compare fundamentally different schemes is indeed important. It is fairly straightforward to determine the accuracy of each scheme depending on the discretisation used as it has been stated in the manuscript. Based on these facts, WENO-5 should be the most accurate scheme as it is 5<sup>th</sup> order in space and 3<sup>rd</sup> order in time, but the high number of particles of MIC allow it to perform really well even though it is 2<sup>nd</sup> order in space, 1<sup>st</sup> order in time for the trajectory tracing and 1<sup>st</sup> order in space for the interpolation step in a similar way as an upwind scheme would perform really well if the resolution was high enough. In that light, what matters is not to fundamentally understand the order of accuracy of each scheme as they are based on fundamentally different approaches but how they perform for realistic geodynamical problems, which is the approach used in this work.

→ New simulations have been performed for a Courant number of 0.7 for testing the extended stability of the MIC and SL; results have been included in the revision.

I was confused by the fact that it was not possible to obtain MIC results using a 128 GB machine for grid resolutions such as 500x1000, when the number of markers is on the order of 10 million.

What was the exact reason for such limit in the current MIC implementation? The final conclusions build on the statement that the MIC scheme lacks mass conservation and it is expensive in terms of computation and memory. I already expressed my concerns about the observed lack of mass conservation in the case of the MIC scheme. I think that it would be also useful if the authors could elaborate more on the computational and memory performance of their MIC implementation.

Response: Unnecessary memory allocations were preventing the MIC to scale well.

→ These issues were solved and multithreading on CPU was implemented on all algorithms to further speed up the computation and allowing to perform all models at high resolution. The figures were updated in the draft with the new results.

Detailed comments:

I. 38 What is exactly the notion of triviality in this case?

Response: The meaning was that it is mathematically well understood.

→ This was clarified in the manuscript.

I. 43 “This brings limitation to the resolution of the model ...” - It is indeed correct that for any given computational resources 1D numerical models can be studied with a higher resolution than 2D models. On the other hand, looking from a 3D physical perspective using approximate 2D numerical models could be considered as relaxing computational limitations to the resolution of the model.

Response: That is correct. We think that 2D models, in particular for two-phase flow in this context should be enough for most cases. But complex 2D models still have computational limitation, in particular if reactive transport wants to be achieved. In this case, it is still important to be able to implement accurate advection schemes.

eq.5 Is it necessary to use the brackets around  $C_e^f$ ?

Response: → The brackets were removed.

I. 84 Perhaps early rather than earlier?

Response: → Corrected.

I. 87 “It consists at tracking individual particles on a Lagrangian frame and to reinterpolate them when needed on an Eulerian stationary mesh grid”. consist at or consist of? to reinterpolate or reinterpolating?

Response: → Corrected to “consist of” and “reinterpolating”.

I. 94 “..to the position of a fixed Eulerian grid..” It would be perhaps worth to mention grid nodes here.

Response: → Corrected.

I. 106 Please change spacial to spatial.

Response: → Corrected.

I. 106 It might be a bit confusing when the term “element” is mentioned here.

Response: → This has been replaced by chemical element

eq. 6 It would be perhaps more transparent if the  $f$  symbol, which stands for fluid, was used in the superscript rather than subscript. It could be mentioned that  $v$  denotes the  $x$  component of the velocity.

Response: To stay consistent with all the other equations used for the schemes, we kept  $f$  as a subscript.

→ The explanation that it represents the  $x$  component of the velocity was added in the manuscript.

I. 109 Please consider using “grid spacing” rather than “increment in space”.

Response: → This has been corrected.

I. 129 Here and in fig. 1 caption, “Upwind” is capitalized, while it is not in I. 111.

Response: → This has been corrected.

I. 129 Please consider removing the comma.

Response: → This has been corrected.

I. 133 Perhaps “for a single grid node” rather than “1 element” would suit better here. This issue reappears in other parts of the manuscript.

Response: → This has been clarified in the manuscript.

I. 153-54: What is meant by “complex problems” here? I suspect that for any problem boundary conditions need a special or careful treatment when a 5-point stencil is used. I don’t think that it is necessary to present in details how BC are treated in this case, but a short description would be useful.

Response: The authors agree that the mention of “complex” boundary conditions is confusing and misleading. Both Neumann and Dirichlet boundaries can be applied with WENO schemes, commonly done by using ghost points. The “complexity” mentioned refers to the fact that, as it is a 5 points stencil, 2 ghost points are required on each side of the model for boundaries other than periodic.

→ This has been clarified in the text and the confusing notion of complexity has been removed.

I. 158 It is not that important, but I’m wondering about the notion of “fully capture” in this case.

Response: This refers to the notion of "shock capture", which often arises from non-linear advection equations such as the Burger equation for example. It means not producing oscillations when dealing with shocks.

I. 164 Please replace spacial by spatial.

Response: → This has been corrected.

I. 171 What is "therefore" referring to?

Response: → This has been clarified in the text.

I. 182 " ... is not easy to determine  $\Delta x$ . A common approach to overcome this limit..." In my view, the term limit may be misleading in this context. I would suggest something like: A common approach to accurately determine ...

Response: → This has been corrected.

I. 193 "a stencil point on the grid" Perhaps it could be described as "a grid node".

Response: → This has been replaced by "grid node".

I. 196 It could be several (neighboring) cells depending on the interpolation order (here cubic, so four nodes are needed to span the interpolation space). On the other hand, it depends on the adopted definition of the cell. Anyway, I think that it would be worth to clarify this issue.

Response: → This was clarified in the manuscript.

I. 214 "...interpolate their values...". Perhaps "...interpolate field values associated with them..."

Response: → This has been corrected.

I. 220 "The initial value of each marker ..." Perhaps "The initial field value in each marker ..."

Response: → This has been corrected.

I. 222-23 The problem of deteriorating marker resolution is not only limited to highly divergent flows. It may also affect incompressible, but strongly stretching flows. In such cases, the density of markers can actually depend on the direction (markers may be locally jammed in a certain direction and rarefied in the direction that is perpendicular). Thus, simple scalar measures of marker density may fail in such cases.

Response: → The idea of this comment has been added to the manuscript.

L. 246-54 In my view, based on the presented description, it is not exactly clear how the field values are interpolated from markers to grid nodes. Is it the least-square type of linear interpolation? How many surrounding cells are used?

Response: The interpolation used is a weighted distance averaging linear interpolant, similar as in Gerya, 2019 for instance using all the markers in the surrounding cells of a grid point  $i$ . We

agree that this was not detailed enough, especially that it is not a conventional interpolant.

→ A detailed explanation with the equations used was added in the manuscript.

I. 256-261 The domain size is given as dimensionless, while the time is in seconds.

Response: → This has been corrected.

I. 268 Isn't  $S_k$  constant for all the internal cells?

Response: It is indeed.

→  $S_k$  was removed from the equation and also on equation 47.

I. 352-354 Is this the description of the ODE solver implemented in DifferentialEquations.jl (I. 348)? Please clarify.

Response: Yes, it is.

→ This has been clarified.

I. 363 The standard deviation is given as a dimensionless quantity, while the size of the model domain is given in meters.

Response: → This has been corrected; SD is also in metre.

I. 366-67 I might be missing something here, but I don't exactly understand how the initial distribution of the melt chemistry is governed. In fig. 8 it appears just bi-modal at  $t=0$  Ma.

Response: The initial distribution of the melt chemistry is indeed bimodal. The initial andesitic composition is a circle of radius of 60 meter.

→ This has been added to the manuscript.

Table 3 Please fix the value of the shear modulus (an incorrect exponent is used).

Response: → This has been corrected.

I. 374-383 This part might be a bit confusing. Although the link to eq. 5 is mentioned in I. 320, I think that it would be useful to clarify which physical fields are advected in this model. Please explain why the oxide content may not be conserved, despite the melt fraction is claimed to be conserved due to the chosen numerical scheme. If the total mass of the melt composition (summed weight percentages?) is renormalized in each time step, then I'm not sure if it could be treated as a conserved quantity.

Response: The melt fraction is equal to the melt filled porosity ( $\phi$ ) in the model, which is solved using Eq. 42 and Eq. 43 using finite differences and TR-BDF2 for the integration in time. This discretization is mass conservative as it is using conservative finite differences. So, the melt fraction is changing through time but not because of eq.5. What is advected by eq. 5 is the mass fraction of oxides  $C_e^f$  in wt%. As we are using a non-conservative equation for the advection,

this mass fraction will not be conserved through time. As the conserved quantity is:

$$\phi \times C_e^f,$$

which represents the mass conservation of the chemical element in the melt (see eq. 4), and we know that the melt fraction is conserved (this was measured in the models), then only the conservation of wt% of the chemical element will be monitored.

The renormalization at each step may indeed prevent it from being considered as a conserved quantity from a theoretical point of view. To test that, the models were also run without the normalisation to see how this impact the mass balance. The results show that this effect is negligible at the modelling scale for all the algorithms (at the order of the 9 decimals for all elements).

→ The part about which field is advected has been clarified in the manuscript.

I. 389 What is meant by mixture here?

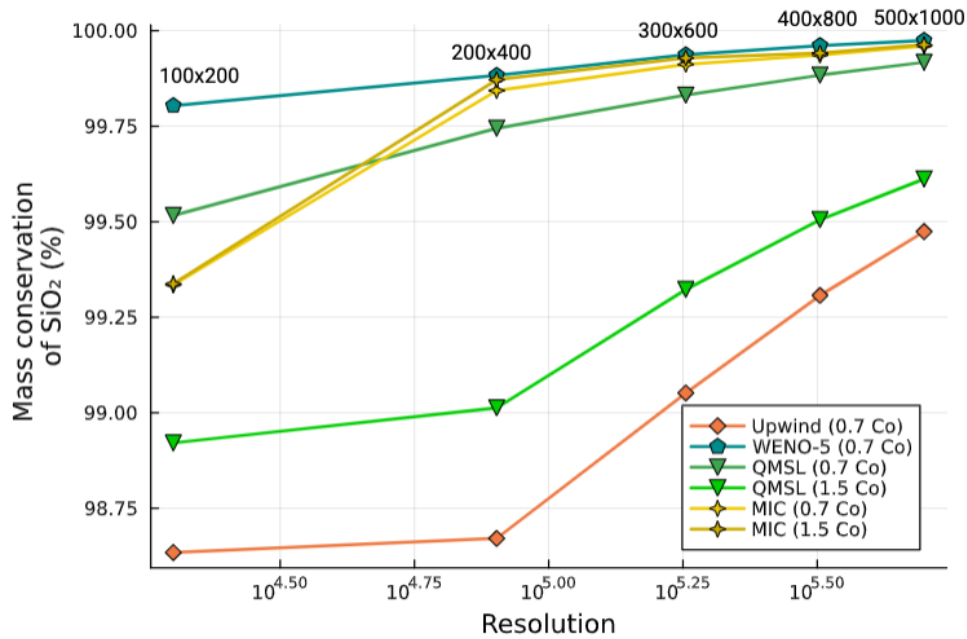
Response: This term is incorrect.

→ Mixture will be replaced by “mixing”.

I. 397 I am a bit confused by the observed lack of mass conservation in the upwind scheme. Is it due to the fact that the renormalization procedure is used? I would also expect MIC to be essentially mass conserving and non-diffusive. Are the observed mass loss effects due to marker reseeding and removal?

Response: The upwind discretization is not mass conservative because we solve a non-conservative form of the advection equation (eq. 5). It will be mass conservative only for simple velocity field and divergence-free. This is shown by the new test added to the revised manuscript. Eulerian methods can only be truly conservative if used on a flux form. The loss of mass of MIC is indeed due to the reseeding and removal, which is not mass conservative. An error was present in the implementation of the scheme, increasing the mass loss.

→ The mention that the upwind discretisation is not mass conservative for divergent flow has been added in the method part, and the MIC implementation error has been corrected in the revision. Here is the new figure obtained:



**Figure 10.** Mass conservation of silica content in the melt fraction for four different advection schemes and five different spatial resolutions at the end of each simulation. The Courant number used is 0.7 for WENO-5 and upwind and 0.7 or 1.5 for QMSL and MIC. The resolutions are 100×200, 200×400, 300×600, 400×800 and 500×1000. The physical parameters used are reported in Table 3.

I. 407 Using mid-point for computing trajectories in MIC and SL results in some iterations.

Response: → This has been corrected.

I. 423 What is exactly meant by complex boundary conditions?

Response: See previous comment on I.153-154.

→ This part will be reformulated in the manuscript.

Fig. 9 & 10 The axes are logarithmic and there is no need to add log(.) in the labels.

Response: → This has been corrected.

References:

Gerya, T. (2019). *Introduction to numerical geodynamic modelling*. Cambridge University Press.