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Geoscientific Model Development Discussions

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Interactive comment on "New strategies for vertical transport in chemistry-transport models: application to the case of the Mount Etna eruption on March 18, 2012 with CHIMERE v2017r4" *by* Mathieu Lachatre et al.

Anonymous Referee #1

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The authors identify three possible options to try and address the issue of excessive vertical diffusion in global, Eulerian, atmospheric models. They test three different solutions: the use of an antidiffusive numerical scheme for vertical transport; increasing the number of vertical layers; and using an alternative scheme to calculate vertical mass fluxes. They find that all three approaches reduce the degree of vertical diffusion, although to different extents. The conclusion drawn is that, while these approaches do not solve the problem of vertical diffusion, some combination of the approach might help to solve this problem.

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I agree fully with the authors that this question is timely, underrepresented in the current literature, and important. The approaches they use are innovative and appropriate, although I have some concerns regarding the results and presentation. With one caveat it appears that the data also generally support the conclusion, which is an incremental but important advance of the conversation surrounding the accuracy of chemistry transport models.

With this in mind, I believe that this paper is also ideally suited for the audience of Geoscientific Model Development. With some revisions, I also believe that it is appropriate for publication. However, there are some concerns I would like to see addressed first.

Major concerns

Firstly, this paper seeks to address two major concerns regarding vertical transport: 1. Vertical transport is poorly represented in most modern chemistry transport modeling efforts, resulting in excessive numerical (and eventually horizontal) diffusion; and 2. The naïve, or brute-force, solution to this – increasing the number of levels in the simulation – is expensive. This paper has done an excellent job of exploring answers to the first question, but does not provide any insight into the second. The two “smart” solutions which the authors propose have their own downsides; the Després and Lagoutière (hereafter DL) advection scheme, while antidiffusive, is also only first-order accurate, while the “directly interpolated winds” (hereafter WRFW) approach violates mass conservation. The utility of the paper would be significantly increased if the authors gave a quantitative assessment of the computational overhead associated with each method and compared it to that associated with the naïve approach. Timing alone, in terms of the number of CPU-hours spent on each simulation, would help with this.

Similarly, the lack of mass conservation in the WRFW approach causes serious concern. I applaud the authors for their frankness in discussing this limitation. However I believe that a full understanding of the advantages and drawbacks of each approach

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demands a fuller discussion of this issue than is currently given in Section 3.2. In Figure 3, it is not clear to the reader why the total domain mass differs so much between each simulation, and it is critically important to the core question of the paper to know why the mass is changing. Specifically, it would help greatly if the authors could quantify on or with Figure 3: 1. How much mass has been (erroneously) lost through the domain upper boundary, based on integrated vertical mass fluxes at the upper boundary; and 2. How much mass has been lost through the domain side boundaries, based on integrated horizontal mass fluxes at the domain boundary. These quantities should enable the authors (and reader) to determine how much of the mass at a given time is spurious, and the degree to which loss through the boundaries is offsetting artificial mass production. On this note, on lines 2-3 of page 14, the authors mention that the "spurious evolutions in tracer mass become weaker, less than 5%" once the plume is more diffuse. Does this really mean "the total domain mass is <105% of the total emitted mass", or is it saying that the amount of mass created spuriously in each time step is <5% of the current domain total? I assume the former, but if so, does this really mean that the error is <5%, or just that the additional spurious mass is now offset by some loss of mass through the domain boundaries?

A broader concern which does not appear to be discussed in detail is the fact that the simulation is driven by fields which are sometimes at a lower vertical resolution. CHIMERE is driven by WRF, running with 33 models, but CHIMERE interpolates this data to its target vertical resolution (Briant et al 2017). Is this interpolation done in a divergence-conserving fashion? If not, does this constitute an uncontrolled-for additional term, in the sense that different vertical grids could introduce different amounts of artificial divergence?

Finally, the authors rely heavily on the trajectory of the plume as a metric of the simulation's fidelity. While the equation to determine error (equation 16) is an interesting formulation, it would be helpful to provide a more quantitative assessment of the amount of numerical diffusion. Variation in the maximum volumetric mixing ratio, the total area of the plume above some minimum VMR, or the total entropy would be useful for quantifying how much numerical diffusion is being introduced. This would also allow the authors to account for the effect that spurious vertical diffusion can have in accelerating spurious horizontal diffusion (relevant papers discussing this issue and metrics of numerical diffusion are e.g. Rastigejev et al 2010, Lauritzen and Thuburn 2012, Eastham et al 2017, Zhuang et al 2018).

Minor comments

I believe that there is an error in equation 15. Using the case of a local maximum (i.e. the first term of the Min operator is negative or zero), the estimated cell boundary VMR ends up being the cell mean VMR + 1, when it should presumably by the cell VMR only (specifically if this is meant to recreate the Godunov donor cell scheme for that condition). Although only a technical error, this is critically important to verification of the rest of the paper.

Section 2.1: it would be helpful to have details on how the vertical layers are placed (i.e. more detail on the different grid discretizations), and where the cell edges lie relative to the WRF vertical grid.

P12 L6: ‘independant’ should be ‘independent’

P18 L21: Currently this line appears to compare the Després and Lagoutière scheme to itself. Should the second instance actually be “van Leer (1977)”?

P20 L2: Why is increasing vertical resolution only meaningful in cases where plume injection altitude is known? I feel that this statement needs to be better qualified. A reduction in numerical diffusion should always correspond to an improvement in simulation fidelity, even if the initial conditions include error.

Finally, the paper has some minor grammatical errors throughout (e.g. page 1 line 15, “The CHIMERE CTM has previously been used to assess Eyjajallajökull eruption possible impact on air quality” should be “..to assess the possible impact of the eruption of

Eyjajallajökull on air quality”). I hesitate to bring these up as the errors are almost always very minor and do not impact the science of the paper, and it is usually possible to determine the authors’ intended meaning. However, these issues do compromise the readability, and as such I would recommend the authors take another sweep through the paper to correct such issues.

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