Answer to Referee #1

Sylvain Mailler[1,2], Romain Pennel[1], Laurent Menut[1], and Mathieu Lachâtre[1]

[1]*LMD/IPSL, École Polytechnique, Institut Polytechnique de Paris, ENS, PSL Research University, Sorbonne Université, CNRS, Palaiseau France*
[2]*École des Ponts-ParisTech, Marne-la-Vallée, France*

We are very grateful of the thorough review performed by the Referee and we would like to thank him for his very encouraging opinion on our work. Due to the useful suggestion of using the same splitting strategy for all numerical experiments to increase confidence in our results, we have redone most of the calculations that were presented. The resulting differences, however, are very small, and do not change the interpretation, strengthening our confidence in the results we present.

We have performed all the changes that were asked by the Reviewer, and believe that the review process has greatly helped us improve our work.

1 Answers to Major comments

> **1. While I understand that the Upwind and DL99 schemes are first-order, it seems like an unnecessary confounding to use different operator splitting methods for these two methods in comparison to the VL and PPM schemes. It would be useful to see a comparison where all schemes are using (e.g.) the Strang operator splitting. Although this is not expected to yield an improvement in the Upwind and DL99 results, it would at least verify that the improved performance is not because of the operator splitting approach. Given the performance characteristics of DL99 (i.e. low sensitivity to small CFL numbers) one would hope that Strangs scheme also would not compromise its accuracy, although it might incur an unnecessary expense.**

We had a discussion among authors on this point before initial submission, and decided to use each scheme "at its best", in the configuration that would be used naturally for a simulation. So, the first-order schemes with a Lie splitting not to incur into excess computational time and not to degrade performance by useless splitting of horizontal time steps, and the second-order schemes with a Strang splitting to preserve their accuracy.

Even though we have been careful to split the horizontal time stepping (which is performed with PPM in all configurations) and not the vertical one, precisely not to lose the ability to compare the runs with each other, we agree with the Referee that this choice adds some uncertainty and may cast doubt on the comparisons we present. Therefore, as the Referee suggests, we have redone the calculations using Strang splitting for all schemes, maintaining the same choice to always split horizontal integration rather than vertical integration. All numbers and plots are changed accordingly in the revised version for the Upwind and DL99 simulations[1]. Below, we introduce and comment the modifications in Tables 3 and 4 brought by this change in the splitting strategy.

	Exact	Upwind	VL	PPM	DL99
Max. MR	30.0	~~6.10~~ **6.11**	10.3	11.7	~~18.5~~ **18.2**
% error (norm 1)	0.	157.	131.	122.	~~87.5~~ **87.6**
% error (norm 2)	0.	86.1	76.9	73.8	~~60.3~~ **60.4**
% mass in envelope	100.0	23.3	39.0	44.6	~~64.7~~ **64.9**

Table 3: Performance of simulations performed with the Upwind, VL, PPM and DL99 vertical advection schemes relative to the discretized exact solution for Case 1: percent relative error in $\|\cdot\|_1$ and $\|\cdot\|_2$ and percent of total tracer mass contained in the correct envelope. The numbers that are not changed up to the third-figure truncature appear in normal fonts, the numbers that are changed appear in bold font, and the former value appears in striked-out font.

	Exact	Upwind	VL	PPM	DL99
Max. MR	100.	24.7	42.2	50.8	~~94.2~~ **92.6**
% error (norm 1)	0.	151.	116.	99.3	~~14.4~~ **18.8**
% error (norm 2)	0.	82.6	69.8	63.2	~~11.2~~ **14.2**
% mass in envelope	100.	24.7	42.0	50.3	~~92.8~~ **90.6**

Table 4: Performance of simulations performed with the Upwind, VL, PPM and DL99 vertical advection schemes relative to the exact solution for Case 2: percent relative error in $\|\cdot\|_1$ and $\|\cdot\|_2$ and percent of total tracer mass contained in the correct envelope. The numbers that are not changed up to the third-figure truncature appear in normal fonts, the numbers that are changed appear in bold font, and the former value appears in striked-out font.

Tables 3 and 4 show that a small part of the improvement obtained by using the Després and Lagoutière (1999) scheme instead of the Colella and Woodward

[1]The numbers for the VL and PPM runs in tables 3-4 were affected by an error (probably due to making these calculations with an earlier model version). The differences presented in tables 3 and 4 of the present document are relative to the corrected values.

(1984) PPM scheme was indeed due to the different splitting approach, as the Referee suggests. This can interpreted as a small amount of additional horizontal diffusion due to splitting horizontal integration. While this additional horizontal diffusion is marginal compared to the strong vertical diffusion in the upwind simulation, it does bring a degradation of a few percents in the performance of the DL99 configutaion, for both simulated cases relative to the Lie splitting. This degradation is however very small compared to the difference between DL99 ans, e.g., PPM, so that the conclusions of the study are not changed.

> **2. It seems like an oversight to not invoke Godunov's theorem (Godunov and Bohachevsky, 1959), especially on lines 306-308. It is a known result that any higher-order scheme cannot exceed first-order accuracy in the vicinity of a sharp gradient, so it is not true that "higher-order schemes are expected to reduce numerical error at any given resolution".**

We are grateful to the Reviewer for drawing our attention to the need for citing the seminal paper of Godunov and Bohachevsky (1959). The result most widely known as Godunov's theorem states that a linear, monotonous scheme, cannot exceed first-order convergence in accuracy. This is why, to ensure monotonicity, higher-order schemes such as Van Leer (1977) or Colella and Woodward (1984), among many others, have to include non-linear "slope limiters" in order to ensure monotonicity, which breaks their linearity.

We have introduced a discussion of our results in light of Godunov's results in the Discussion section.

> **3. On line 327, the authors state that "if model resolution is fine enough to represent properly the plume, then higher-order schemes are still a better choice", but I am not sure this is true (or that this manuscript even supports that conclusion). An important point they raised is that the DL99 scheme does a good job even in the situation of low CFL numbers (line 140), and it seems that such conditions are likely to be common when considering vertical movement in the atmosphere. I would recommend that this conclusion be removed or at least made more precise to account for the fact that it may only be true under certain conditions. This is hinted at through the final sentence of the discussion (line 318) but the authors are understating the importance of this point. The implication that increasing vertical resolution may be an inefficient solution for even higher-order methods is a potentially significant finding.**

The missing point in the lines that are cited is that the statements such as "if model resolution is fine enough to represent properly the plume, then higher-order schemes are still a better choice" are true if the underlying tracer field is smooth. In this case (and only in this case), theory guarantees that if the resolution is fine enough, then error becomes smaller for higher-order schemes. In presence of shocks in the tracer concentration and/or its derivatives, such statements are false.

The discussion section has been rewritten in more detail to take into account the elements raised by the Referee.

2 Answers to Minor comments

> **1. Figures 1 and 2 would be improved by using the same color scale for all panels (i.e. 0-20 ppb for Figure 1, and 0-100 ppb for Figure 2)**

The colorscales have been changed as the Reviewer suggests (improving read-

ability)

> **2. I would suggest that the authors consider replacing promising novelty in the title with, say, promising and novel solution to . I think that novelty makes the work sound unimportant, whereas I found this work to be intriguing and of high value.**

We would like to thank the Referee for his very encouraging appreciation on our manuscript. For the revised version we propose the following title (also taking into account the comment from the Executive Editor requesting that the scheme we refer to shall be named in the title):

Using the Després and Lagoutière (1999) antidiffusive transport scheme: a promising and novel method against excessive vertical diffusion in chemistry-transport models.

3 Typos

Finally, I tried to make a note of any typos or grammatical errors I found. However, I would suggest that the authors make an additional sweep for grammatical accuracy:

1. Line 9: "an important direction into improvemen" doesn't quite make sense. Perhaps "necessary step in the development"?

Changed accordingly.

2. Line 17: “too much observations” should be “too much compared to observations”

Changed accordingly.

3. Line 72: “permit” should be “ensure” or similar

Changed accordingly.

4. Line 73: there is a spurious space between the closing bracket and comma.

Space has been removed.

5. Figure 3 caption: “shox” should be “show”

Changed accordingly

6. Line 309: “teh” should be “the”

Changed accordingly (line 309 and in another occurence)

7. Line 328: “enaugh” should be “enough”

Changed accordingly

8. Line 336: “adress” should be “address”

Changed accordingly (line 336 and in another occurence)

9. Throughout: 1d should be 1D or 1-D

Changed accordingly

10. Throughout: some language is somewhat nonscientific (e.g. spectacular on line 298 is hyperbolic)

Spectacular has been replaced by “substantial” (and the sentence has been rephrased).

We have re-read thoroughly the document and tried, as suggested, to improve some formulations and vocabulary.

4 References

References

Colella, P. and Woodward, P. R.: The piecewise parabolic method (PPM) for gas-dynamical simulations, Journal of Computational Physics, 11, 38–39, 1984.

Després, B. and Lagoutière, F.: Un schma non linéaire anti-dissipatif pour l’équation d’advection linéaire, Comptes Rendus de l’Académie des Sciences - Series I - Mathematics, 328, 939 – 943, https://doi.org/https://doi.org/10.1016/S0764-4442(99)80301-2, URL http://www.sciencedirect.com/science/article/pii/S0764444299803012, 1999.

Godunov, S. K. and Bohachevsky, I.: Finite difference method for numerical computation of discontinuous solutions of the equations of fluid dynamics, Matematičeskij sbornik, 47(89), 271–306, URL https://hal.archives-ouvertes.fr/hal-01620642, 1959.

Van Leer, B.: Towards the ultimate conservative difference scheme. IV. A new approach to numerical convection, Journal of Computational Physics, 23, 276

– 299, https://doi.org/https://doi.org/10.1016/0021-9991(77)90095-X, URL `http://www.sciencedirect.com/science/article/pii/002199917790095X`, 1977.