Answer to the Reviewer Comment signed by Christopher Walcek 10.5194/gmd-2023-78-RC1 on the manuscript "**An improved version of the Piecewise Parabolic Method advection scheme: description and performance assessment in a bidimensional testcase with stiff chemistry in toyCTM v1.0.**"

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July 28, 2023.

We are grateful to Christopher Walcek for his careful reading and insightful comments on our manuscript. Two main comments by Pr. Walcek regard the need to discuss how a higher-resolution would affect our results, and the question of the "inability to preserve lumped but conserved species". We address both these comments in detail below.

Contents

1 Comments by C. Walcek

The authors introduce a modification and improvement of numerical advection algorithms by merging existing techniques in a way the optimizes the numerical approximation of advection. They also introduce a new error metric that assesses not only local extrema, but also the distribution and range of concentration distributions that are advected. My main complaint about the study is the limited nature of the test presented (only one Courant number, and one fairly well-resolved gaussian hill shape. Aside from a few minor pounts that need to be mentioned, the paper is publishable.

1. typo line 250. How can fluid density everywhere be zero. is this a typo ?

2. using these deformational flows, figures like 8c and others do not properly quantify the true "accuracy" of the scheme since the shape is advected/sheared into a shape that has scale features that are smaller than the 4 km resolution of this experiment. If this entire study were performed at 1 or 0.1 km resolution, the error measures would change. Basically, the simulation called "base" in these figures is not a true average of the 4x4km resolution "base". When the peak of the "base" Guassuan shape is sheared into successively smaller and smaller cells, then averaged BACK to the 4 km coarse T=0 4km-resolution discrete grid, then the simulation called "base" should change with time also. This applies to the figures which show the distribution at the T/2 times at the point where the. Here the authors could do a simulation at spatial resolution of 0.4 km (much smaller than 4 km), then MAP the 0.4 km simulation back onto the 4km "base" grid by averaging 10X10 grid cells into a single 4 km grid, then compare.

3. one of the problems with the Walcek peak scheme is the inability to preserve lumped but conserved species since there it is guaranteed that numerical treatment around local maxima are NOT treated identical

	Normalized $\|\cdot\|_1$ error				$\mathcal{E}_1$			
	TRC	O3	NO2	NO	TRC	O3	NO2	NO
Godunov	0.434	0.275	0.357	0.584	0.386	0.244	0.237	0.564
Van Leer	0.0417	0.0486	0.0521	0.0905	0.0241	0.0418	0.0325	0.0773
Walcek	0.0202	<u>0.0303</u>	0.0423	<u>0.0509</u>	0.016	0.0244	0.0344	0.0472
PPM	<u>0.0169</u>	0.0336	**0.0324**	0.0574	**0.00881**	<u>0.0221</u>	**0.0263**	<u>0.0382</u>
PPM+W	**0.0148**	**0.0247**	<u>0.0383</u>	**0.0483**	<u>0.00901</u>	**0.0112**	<u>0.031</u>	**0.0332**

Table 1: Normalized $\|\cdot\|_1$ error E_1 and normalized $\|\cdot\|_1$ signature error $\mathcal{E}_1$ **in the 1 km simulations** at the end of the simulations for O_3, NO, NO_2 and TRC, compared to the Base simulation with no advection. In each column, the lowest error value is in bold font, the second-lowest in underlined.

in SUMS of conserved species. The "peaks" in NO, NO_2 and HNO_3 will occur at different places than the combined NO+NO_2+HNO_3. In the context of the problem presented here, total nitrogen should be conserved (NO+NO2+HNO3). The authors should be able to show that there is non-monotonic behavior of any advection scheme which treats local EXTREMES algebraically differently. Please show graphs of NO+NO_2+HNO_3.

2 General answer

Pr. Walcek judges this paper publishable, with one main complaint about "the limited nature of the test presented (only one Courant number, and one fairly well-resolved gaussian hill shape)".

We agree that the fact that there is only one test presented could be a limit, however the manuscript presents objective scores for two different metrics and 4 different species on a total of 5 simulations, amounting to 40 metric scores, and these different species test the advection schemes in different conditions because their distributions are very different. We also introduce one new advection scheme (that has to be explained) and a different metric with the idea, as Pr. Walcek describes it, to assess "not only local extrema, but also the distribution and range of concentration distributions that are advected". This has guided the choice to perform only one test-case (but with several advection configurations and chemical species).

It is true that there is "only one Courant number", which does evolve in time though since the mass-flux (and therefore the CFL) is equal to zero at $\frac{T}{2}$. For the same reasons as above, we did not perform a sensitivity test on timestep.

These limits/questions will be acknowledged in the manuscript for a revised version.

Regarding the fact that our test case consists essentially of a "fairly well-resolved gaussian hill shape", this is essentially true for the inert tracers, even at half-time under the influence of wind shear (Fig. 5 of the manuscript), but this is not true for the ozone concentrations. Fig. 6 of the manuscript (reproduced here as Fig. 1) shows that the high-ozone belt that circles the plume takes an extremely elongated shape under the effect of wind shear and of the different chemical regimes. Fig. 1 clearly shows that this high-ozone belt has a croos-dimension of the order of magnitude of one single grid-cell, which is extremely challenging for the advection framework.

3 Specific answers

On point **1.**, equation $\rho(x;y;z;t=0)$ is not properly written, as the Reviewer indicates. "a fluid with density $\rho(x;y;z;t=0)$" will be replaced by "a fluid with density $\rho(x;y;z;t)$", since we do not refer specifically to the initial density at this point, so that our formulation causes confusion..

3.1 On the resolution

On point **2.**, it is true that "if this entire study were performed at 1 or 0.1 km resolution the error measures would change". Even though we did not understand the exact procedure suggested by the Reviewer, we did perform the same simulation set at 2 km and 1 km resolutions. We provide here in Table 1 the equivalent

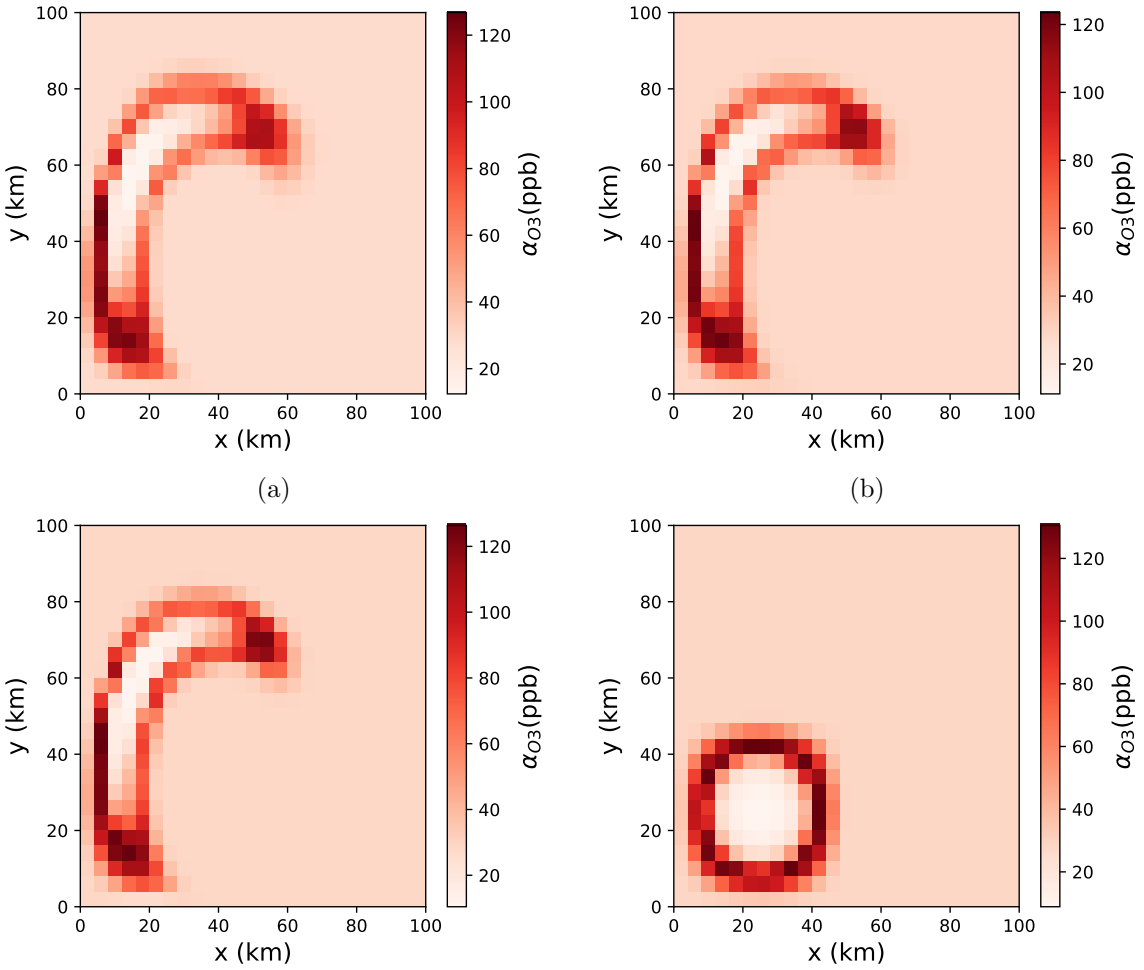
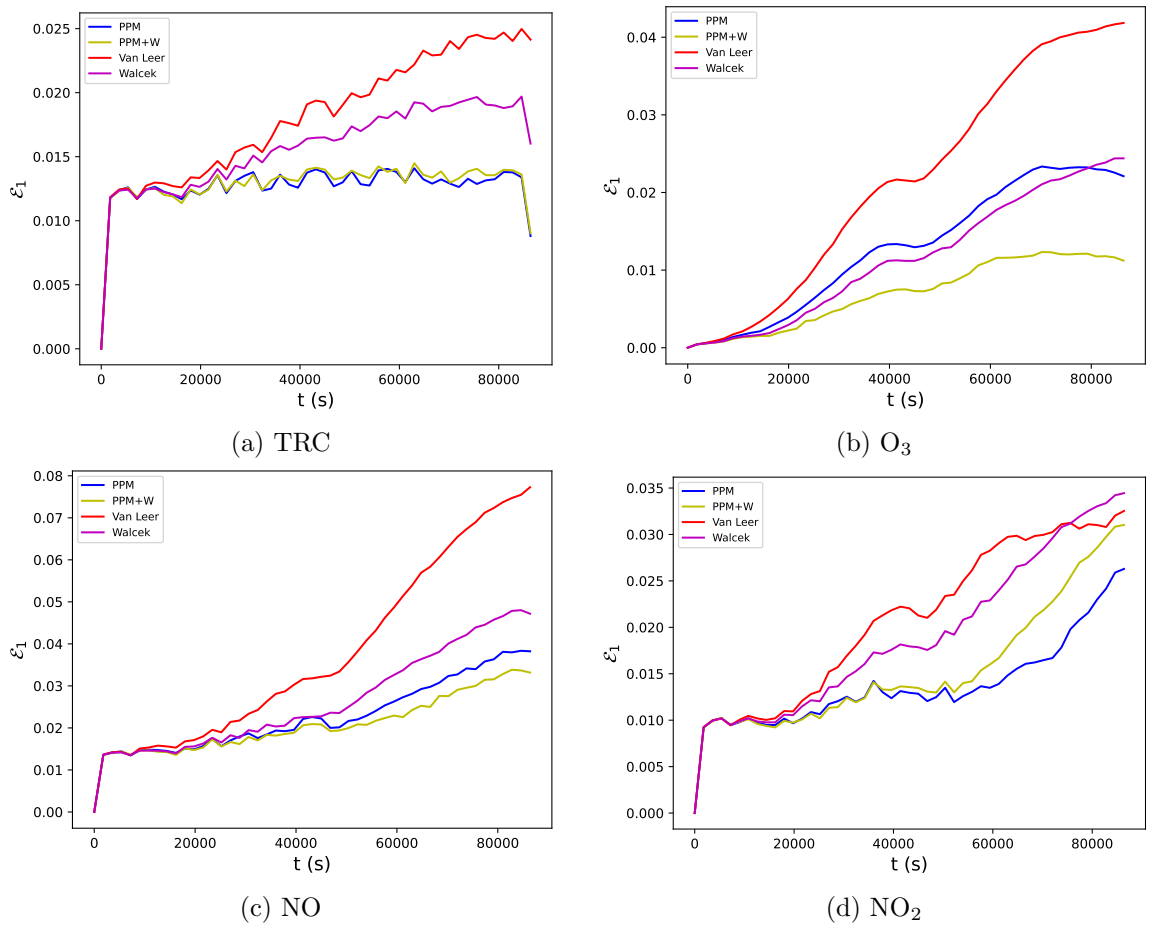


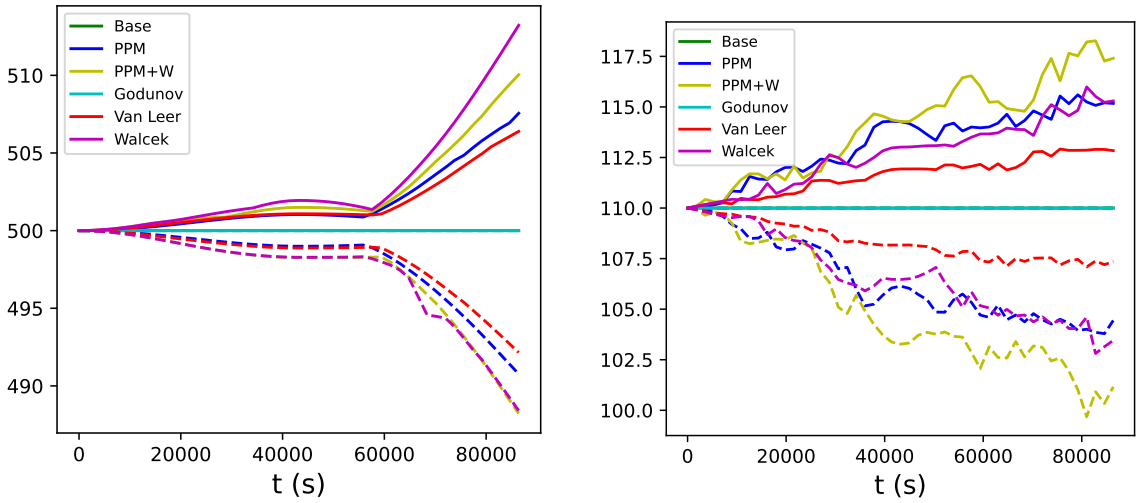
Figure 1: Ozone mixing ratio at $\frac{T}{2}$ as simulated in (a) the Van Leer simulation; (b) the PPM simulation, (c) the PPM+W simulation and (d) the Base simulation.



(a) TRC (b) O_3

(c) NO (d) NO_2

Figure 2: Time series for $\mathcal{E}_1$ ($\|\cdot\|_1$ normalized signature error) **the 1 km resolution simulation** for (a) TRC; (b) O_3; (c) NO and (d) NO_2



(a) (b)

Figure 3: Minimum and maximum values in the 4 km simulations (presented in the manuscript) for: $\alpha_{CO} + \alpha_{CO_2}$ (panel (a)) and $\alpha_{NO} + \alpha_{NO_2} + \alpha_{HNO_3} + \alpha_{TRCb}$ (panel (b))

of Table 4 in the manuscript, for the same simulation but with 1 km resolution instead of 4 km, keeping the same Courant number (the time step is therefore also divided by 4 compared to the 4 km simulation, from 1800 s to 450 s).

The results are relatively consistent with the results shown in the manuscript, even though at this high resolution the performance of PPM improves relative to the Walcek scheme. At 4 km resolution, the PPM+W scheme was performing best for all species, but at 1 km the PPM scheme performs comparably for inert tracer TRC, and better for NO_2, while PPM+W performs better for O_2 and NO. Also, while at 4 km resolution the Walcek scheme was performing better than PPM for all species except O_3, the performance of PPM seems to improve faster than that of the Walcek scheme with increased resolution, consistently with the third-order design of the PPM scheme compared to second-order for the Walcek scheme.

While at 4 km resolution the PPM+W scheme was clearly and consistently outperforming all the other tested schemes, this is not the case at 1 km resolution, where it is clearly outperformed by the classical PPM scheme for one variable. However, even at this 1km resolution, the PPM+W scheme has the most consistent and robust performance, being either first or second in the comparison for all the variables and criteria.

Fig. 2 is the equivalent of Fig. 9 in the manuscript but with $\delta x = 1\,\text{km}$, and shows the evolution in time of the $\mathcal{E}_1$ error in the various simulations for TRC, NO, NO_2 and O_3 respectively. It gives a vision of the time evolution of error along the run, confirming the extremely similar behaviour of PPM+W and PPM with regards to inert tracer TRC throughout the simulation (Fig. 2a), the equivalent or slightly better performance of PPM+W compared to PPM regarding NO throughout the run, and the better performance of PPM+W on O_3 throughout the run. The time series regarding NO_2 is more interesting, since we see that during the first half of the simulation the PPM+W run performs similarly to PPM, but in the second half the error increases faster, bringing PPM+W at error levels close to those of the Van Leer and Walcek schemes for this variable.

These additional results for higher resolution will be commented in the revised version if we are invited to submit one.

3.2 On the conservation of sum species

On point **3.**, we do not think this problem is specific to the Walcek time scheme. Apart from the Godunov donor-cell model, all other advection schemes in our study are non-linear. This is linked to the Godunov theorem, which states that there exists no linear and monotonous order-2 advection scheme, so that all the order-2 (and higher) schemes used in practice (and in our study) are non-linear, due to the use of slope-

limiters. With these nonlinear slope limiters, if two species initially have a uniform sum, this uniformity will be lost during the run. Assessing such effects with the sum $NO + NO_2 + HNO_3$ is difficult since the sum is not initially uniform (it follows the Gaussian shape of Fig. 2 of this manuscript). To assess the magnitude to these undesirable effects with the various advection schemes we use here, **we have performed the same simulations with a new tracer species TRCb** so that initially we have $\alpha_{NO} + \alpha_{NO_2} + \alpha_{HNO_3} + \alpha_{TRCb} = 110\,ppb$. We present the maps of $\alpha_{NO} + \alpha_{NO_2} + \alpha_{HNO_3} + \alpha_{TRCb}$ at the end of the experiment, and the time-series of the minimum and maximum of $\alpha_{NO} + \alpha_{NO_2} + \alpha_{HNO_3} + \alpha_{TRCb} = 110\,ppb$. We also present the time series for $\alpha_{CO} + \alpha_{CO_2}$ which, in our study, should be constant, uniform and equal to 500 ppb everywhere in an exact solution, but is not for the same non-linearity reasons as with nitrogen.

Several elements can be inferred from Figure 3a-b:

- As expected, the linearity of the Godunov donor-cell scheme allows it to preserve exactly the uniform sum of two or several species with non-uniform distribution. In conformity with the Godunov theorem, higher-order schemes do not.
- Departure of the modelled sum compared to its expected values are up to ±3% for C and up to ±3% for N.
- Apart from the Godunov scheme, the Van Leer scheme is the least affected by this phenomenon, while the Walcek and PPM+W schemes are the most affected.

To verify that these discrepancies are indeed due to the treatment of the extrema, we provide maps of $\alpha_{NO} + \alpha_{NO_2} + \alpha_{HNO_3} + \alpha_{TRCb}$ at the end of the simulation (Fig. 4). These maps show that the discrepancies are indeed stronger in the vicinity of the peak of NO_x mixing ratios, and that the error patterns are extremely similar in all schemes.

Fig. 3 will be included in a revised version of this manuscript if we are invited to submit one.

With our best regards,

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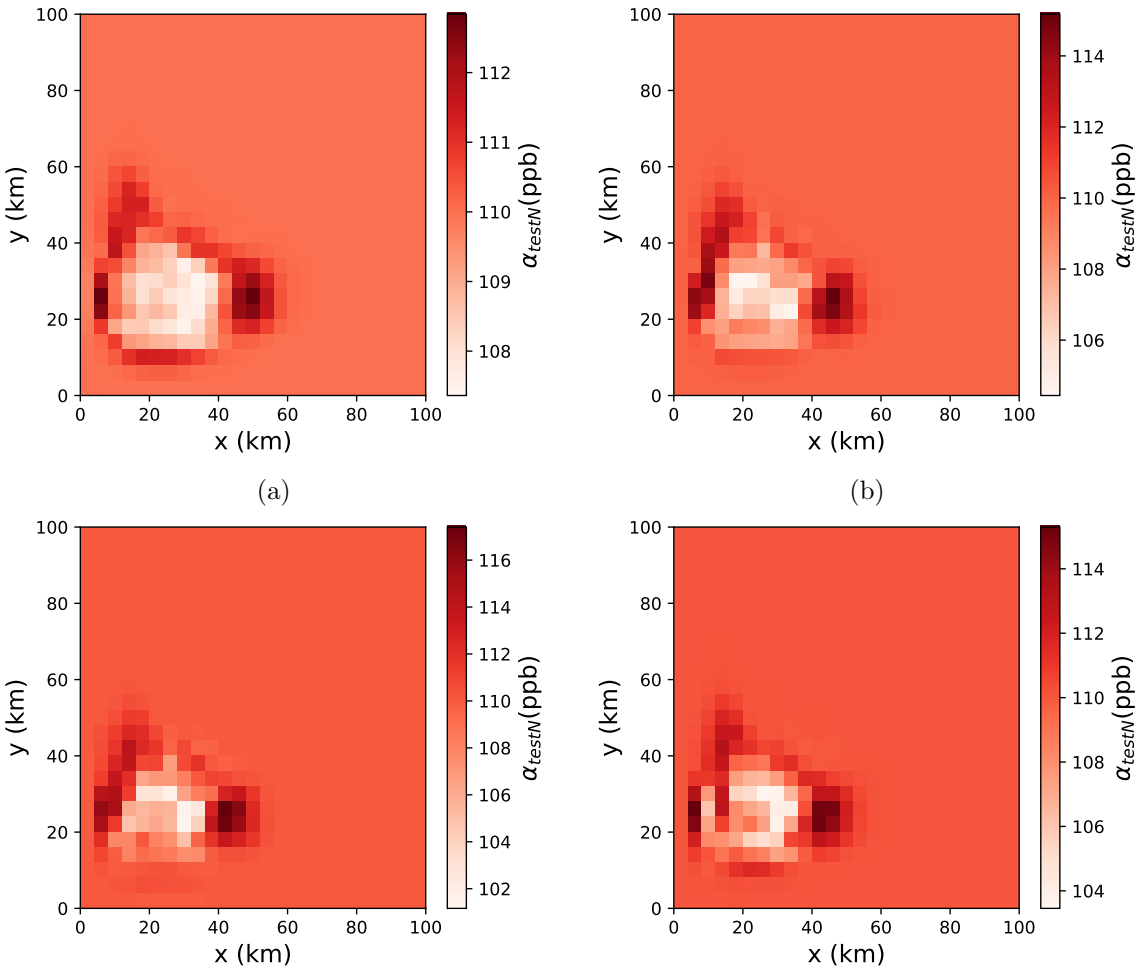

Figure 4: $\alpha_{\mathrm{NO}} + \alpha_{\mathrm{NO_2}} + \alpha_{\mathrm{HNO_3}} + \alpha_{\mathrm{TRCb}}$ at $t = T$ as simulated in (a) the Van Leer simulation; (b) the PPM simulation, (c) the PPM+W simulation and (d) the Walcek simulation.