

Answer to RC2 Anonymous Reviewer#2 10.5194/gmd-2023-78-RC2 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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We are grateful to Anonymous Reviewer#2 for their careful reading and insightful comments on our manuscript. The main comments by Anonymous Reviewer#2 regard the need...

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## 1 Comments by Anonymous Reviewer#2

### 1.1 General comments

The authors integrated PPM with the flux adjustment of Walcek method to improve the representation of local extrema which results in overall improvement without an increase in computational intensity. To evaluate their method they performed a simulation with different advection schemes with a chemical mechanism. They introduced the signature function as an alternative error statistic which basically evaluates whether the concentration probability distribution remains unchanged after advection. I think the advection scheme they suggested here is certainly an advancement for chemical transport modeling but the way they evaluated the method is in question.

The chemical transport model deals with the various velocity fields and initial conditions. I don't think the authors need to test their model with very realistic data, but just one simulation is not sufficient. For example, the key advancement of their method is on how to address local maxima, but there is only one local maxima in their initial condition. I'm curious how much the method will be effective if there are more stiff gradients—even testing with those scenarios can give them more benefits in computational cost.

They alleged that theoretically, the signature function will remain the same if there is no numerical error. I think they can change if the wind field has divergence. For example, if there is a negative divergence in a certain region, the concentration can be accumulated and the number of cells with high concentration can increase and the maximum range can increase. In case of the positive divergence, the wind will make scalars dispersed away so the number of cells with low concentration increases and the number of high concentration cells will decrease. The negative divergence scenario is relevant to high pollution episodes trapped by temperature inversion like LA smog while the positive divergence scenario is like the radial spread of volcanic ash. Even though those might be a bit extreme cases, it is the role of a chemical transport model to address those cases and in this regard the signature function cannot guarantee a proper evaluation.

If authors admit that the signature function works well on non-divergent wind scenarios including their simulation here, then it can make sense. However, the assertion that the function as a good method working universally is not true in my opinion.

## 1.2 Minor details

Below are minor details authors can correct:

L75 typo: ... the three reactions wthat ...

L80-90: R3 and R8 are incorrect in stoichiometry

Table 1: mean with standard deviation will be better to represent execution time

L256: The variable X should be explained.

Equation 11: H is non-italic here but in L259 it's italic.

L264: X is non-italic here.

L300: This sentence does not make sense to my perspective as I explained above.

L320: For similar reason, I don't think the maximum or minimum will not change. It is more natural to evolve with time when there is divergence.

L334: There might need a period in the middle. Looks like two different sentences are not properly separated.

L361: performace looks like a typo of performance

L364 365: The conclusions drawn from the analysis... but the evidence is only a single experiment?

L375: Is a signature function really invariant? (same for other invariants authors mentioned)

## 2 Answer to the General comments

**Anonymous Reviewer#2** : "The chemical transport model deals with the various velocity fields and initial conditions. I don't think the authors need to test their model with very realistic data, but just one simulation is not sufficient. For example, the key advancement of their method is on how to address local maxima, but there is only one local maxima in their initial condition. I'm curious how much the method will be effective if there are more stiff gradients—even testing with those scenarios can give them more benefits in computational cost."

**Answer**: While it is true that only one local maximum exists in the initial condition (for tracers and nitrogen oxides), this is a testcase with active chemistry. And with the chemical evolution of the system, other configurations appear along the test for species with active chemistry. For example, ozone evolves into an absolute minimum of mixing ratio surrounded by a thin belt of high values then decreasing towards te background value away from the plume (Fig. 6 of the manuscript (reproduced here as Fig. 1)). The initially bell-shaped maximum for inert tracers also evolves into a curved, elongated shape (Fig. 5 in the manuscript). The chemical evolution of concentrations does generate very stiff gradients. For example, Fig. 1 clearly shows that this high-ozone belt has a cross-dimension of the order of magnitude of one single grid-cell, which is extremely challenging for the advection framework.

**Anonymous Reviewer#2** : They alleged that theoretically, the signature function will remain the same if there is no numerical error. I think they can change if the wind field has divergence. For example, if there is a negative divergence in a certain region, the concentration can be accumulated and the number of cells with high concentration can increase and the maximum range can increase. In case of the positive divergence, the wind will make scalars dispersed away so the number of cells with low concentration increases and the number of high concentration cells will decrease. The negative divergence scenario is relevant to high pollution episodes trapped by temperature inversion like LA smog while the positive divergence scenario is like the radial spread of volcanic ash. Even though those might be a bit extreme cases, it is the role of a chemical transport model to address those cases and in this regard the signature function cannot guarantee a proper evaluation.

**Answer**: We maintain that, in the absence of mixing, the signature function is strictly preserved by the

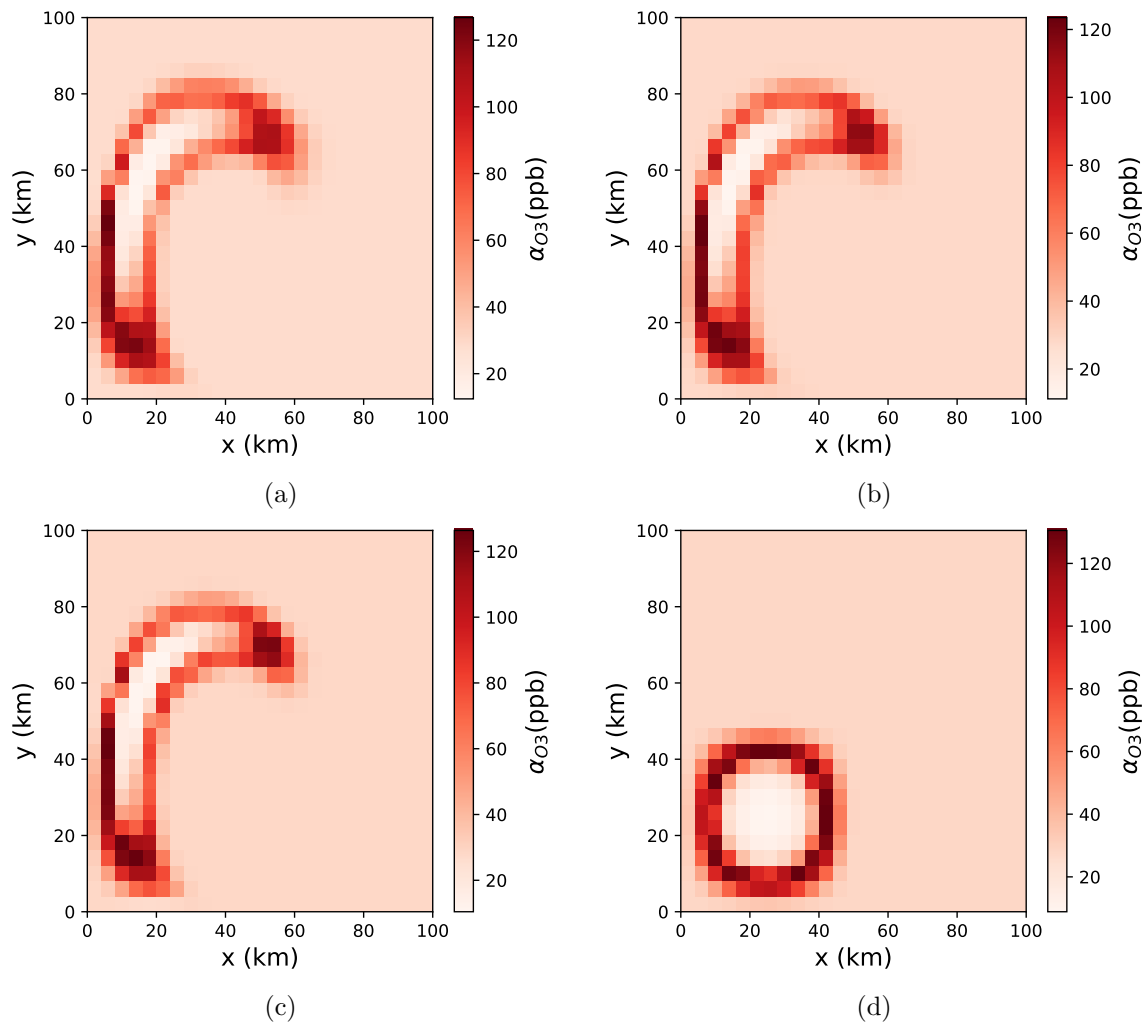


Figure 1: Ozone mixing ratio at  $\frac{T}{2}$  as simulated in (a) the Van Leer simulation; (b) the PPM simulation, (c) the PPM+W simulation and (d) the Base simulation.

advection equation—Eq. 10 in the initial manuscript, reproduced here as Equation. 1:

$$\frac{\partial \alpha}{\partial t} + \mathbf{u} \nabla \alpha = 0. \quad (1)$$

The proof for this is given from lines 264-269 of the manuscript along with Eq. 11, which formally defines the signature function—reproduced here as Eq. 2:

$$\mathcal{S}^t(X) = \frac{\int_{\mathcal{D}} \mathbf{H}(X - \alpha(x; y; z; t)) \rho d\mathcal{V}}{\int_{\mathcal{D}} \rho d\mathcal{V}}, \quad (2)$$

. It is true that, as the Reviewer says, the convergent (resp. divergent) character of the wind field will increase (resp. decrease) the *concentration* of an inert tracer along a trajectory, but it will leave unchanged its *mixing ratio*, which is the key point in constructing the signature function and showing that it is, indeed, invariant under the action of pure advection.

Equation 2, defining the signature function  $X \mapsto \mathcal{S}(X)$ , is constructed as a ratio. Both the numerator and the denominator of this ratio are constant in time due to the specific properties of the advection equation and the continuity equation (Eq. 9 in the manuscript), and this holds even if the wind field has a divergence:

- Numerator,  $\int_{\mathcal{D}} \mathbf{H}(X - \alpha(x; y; z; t)) \rho d\mathcal{V}$ , represents the mass of fluid contained in fluid parcels with tracer mixing ratio  $\alpha(x; y; z; t) < X$ . This is constant in time (for any value of  $X$ ) because the mass of any fluid parcel is constant in time (this is a property of the continuity equation), and the tracer mixing ratio in any fluid parcel is also constant in time (this is a property of the advection equation, Eq. 1).
- Denominator,  $\int_{\mathcal{D}} \rho d\mathcal{V}$ , represents the total mass of fluid (e.g., air), which is preserved if there is no flux across the domain boundary, which is essentially the case of, e.g., the entire atmosphere, or if the fluid moves within a “box” as in our academic case.

Therefore, the signature function  $\mathcal{S}$  is rigorously invariant under the action of the advection equation, even in the case in which the wind field is divergent.

This is true of the complete, formal definition shown in Eq. 11. in the manuscript. Eq. 12 shows how this definition can be discretized to test the properties of numerical advection schemes in a Eulerian model without loss of generality (including the case of a divergent wind field). Equations 13-14 in the manuscript is just a practical “trick” to calculate very easily the signature error in the particular case where every cell of the model contains the same mass of fluid, and this mass of fluid does not vary in time. While is already said in the manuscript that this “trick” applies only “in the particular case in which the carrier fluid mass  $\rho_i V_i$  is the same in all model cells”, which is true throughout time only for non-divergent fluxes.

✓ the comment by Anonymous Reviewer#2 shows that a clarification of which quantities are invariant even in divergent fluxes, and which quantities are not would be helpful in the text. Explicit statements in this sense have been included in Section 4.2..

**Anonymous Reviewer#2** : If authors admit that the signature function works well on non-divergent wind scenarios including their simulation here, then it can make sense. However, the assertion that the function as a good method working universally is not true in my opinion.

**Answer**: We do not assert that the signature function is working universally. However, in the conclusion, we will precise the range of applicability of the invariance of the signature function for realistic applications. While, as discussed above, the invariance of function  $\mathcal{S}$  holds in the presence of divergence, it applies only to pure advection problems, excluding the presence of diffusion and mixing.

✓ These precisions are brought into the conclusion in the revised version of the manuscript in order to better specify and discuss the possible applicability of the signature function as an invariant in realistic problems.

### 3 Specific answers

**Anonymous Reviewer#2** :L75 typo: ... the three reactions wthat ...

✓ Corrected

**Anonymous Reviewer#2** :L80-90: R3 and R8 are incorrect in stoichiometry

**Answer:** The fact that R8 is not balanced in stoichiometry is due to the omission of O<sub>2</sub> as a reactant, as explained in lines 220-223 in the manuscript. The imbalance it introduces in the system is only on dioxygen, it is common practice in atmospheric chemistry to ignore such imbalances because they do not affect measurably the amount of oxygen available. Introducing this formally imbalanced reaction saves computation time by avoiding to introduce atomic hydrogen H as an intermediary species.

The incorrect stoichiometry in reaction R3 is also due to the omission of O<sub>2</sub>, this time as a product. This is also common practice in chemistry-transport modelling for the same reason as above, but

✓ **consistently with reactions R4, R7, R10 and R11, O<sub>2</sub> will be included in the products list in the revised version.**

**Anonymous Reviewer#2** : Table 1: mean with standard deviation will be better to represent execution time

**Answer:** As shown by Table 1, the execution time for one call to the advection routine is a few dozen nanoseconds at max. the system clock we could access for this benchmark has a time step of 1 ms, which is why we have run each of the schemes  $1.04 \times 10^8$  times (line 183) to evaluate the calculation time for one call. With this method, we are able to evaluate the average time but not its distribution, and we do not see a way to go beyond this limit. The initial caption of Table 1 may suggest that the execution time for the schemes is constant regardless of the input values, which is not the case due to the conditional statements in the schemes.

✓ **In the revised version, we make clear that the value we give is an average by writing “Mean calculation time” instead of “Calculation time”.**

**Anonymous Reviewer#2** :L256: The variable X should be explained.

**Answer:** X is a dummy variable used only to define function  $\mathcal{S}$ .

✓ **we have clarified the meaning of X in the revised version:** For any given time  $t$  and any mixing ratio  $0 \leq X \leq 1$ , we can define  $\mathcal{S}^t(X) \dots$

**Anonymous Reviewer#2** : Equation 11: H is non-italic here but in L259 it's italic.

**Answer:** ✓ **Fixed, thanks**

**Anonymous Reviewer#2** :L264: X is non-italic here.

**Answer:** ✓ **Fixed, thanks**

**Anonymous Reviewer#2** L300: This sentence does not make sense to my perspective as I explained above.

**Answer:** We are not able to understand this concern, and do not see any reference to this in the above comments, sorry.

**Anonymous Reviewer#2** L320: For similar reason, I don't think the maximum or minimum will not change. It is more natural to evolve with time when there is divergence.

**Answer:** The minimum and maximum of the mixing ratio (not of the concentration) have to stay constant in time even in the presence of divergence, *per* Eq. 1 which shows that the mixing ratio has to stay constant along any trajectory (this equation holds even if the wind field is divergent).

**Anonymous Reviewer#2** L334: There might need a period in the middle. Looks like two different sentences are not properly separated.

**Answer:** there was a point missing in the middle,

✓ **it has been fixed, thank you.**

**Anonymous Reviewer#2** L361: performance looks like a typo of performance

**Answer:** ✓ **it has been fixed, thank you.**

**Anonymous Reviewer#2** L364 365: The conclusions drawn from the analysis... but the evidence is only a single experiment?

✓ We have added to the conclusion additional discussion on the relevance and possible limits of our conclusions, including the fact that they rely mostly on one test-case. Also, the revised version presents more numerical experiments to mitigate this limit, including a convergence test and a higher-resolution simulation.

**Anonymous Reviewer#2** L375: Is a signature function really invariant? (same for other invariants authors mentioned)

**Answer** As discussed above, we feel that we have proved that the signature function is really an invariant

(see the discussion above). Also, the minimum and maximum of tracer mixing ratio are indeed invariants in the advection equation (unlike maxima and minima of tracer density) as discussed in, e.g., Brasseur and Jacob [2017] : “For a constant velocity, the advection of both the density and the mixing ratio is represented by a simple translation (without deformation) of the initial function in the direction of the velocity. If the velocity decreases with space, the initial distribution of both quantities is distorted as the material is advected. The value of the maximum mixing ratio is unchanged, but the maximum value of the density is enhanced. Advection can thus modify extrema of tracer densities in a diverging flow.”

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## References

G. P. Brasseur and D. J Jacob. Chap. 7, numerical methods for advection. In *Modeling of atmospheric chemistry*. Cambridge University Press, 2017.