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Geoscientific Model Development Discussions

Interactive comment on "The terminator "toy"-chemistry test: a simple tool to assess errors in transport schemes" *by* P. H. Lauritzen et al.

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Below the reviewer comments are in black font and author reply in blue font:

That pesky chemistry – when perfect chemistry and perfect transport collide. The authors highlight a very important problem facing chemistry-transport modeling. One that is discovered by most model developers, solved or pasted over, and often buried without publication as it hardly counts as 'science'. I owe the descriptive title above to long-ago discussions with Anne Douglass. This topic should be investigated and highlighted in a GMD paper so that the community can learn from these experiments and hopefully build more accurate chemistry-transport models. This paper is well written

overall and should be published in GMD after minor revisions. There are some discussion sections that need a broader perspective, and some technical sections that do not really help the reader understand the general importance of the work.

We thank the reviewer for reviewing the manuscript and providing very useful comments. The revised manuscript is available in the supplement.

Abstract (L9) – This statement about Cl-y being a conserved quantity is factually incorrect. In 1990 Prather and Jaffe (1990 JGR, "Global impact of the Antarctic ozone hole - chemical-propagation") examined the very large gradients (as in the toy chemistry here) at the chemical front between Antarctic ozone hole air and ambient mid-latitude air. Non-conservation of Cl-y was generated at this front because of differential molecular diffusion. Other studies like Edouard, Legras et al. (1996 JGR, "The effect of dynamical mixing in a simple model of the ozone hole") also looked at the microstructure of chemical species across such gradients. This is a real phenomenon and would clearly apply to the Cl and Cl2 which would have different diffusivities. Nevertheless the models being tested here do not get down to the 10s of meters scale and do not include such diffusion, so they should conserve Cl-y. The design and tests here are correct for the global chemistry transport models, but the authors should recognize that as one goes to finer scales, expect different behavior.

Agreed

Changes to the manuscript: Statements to clarify and highlight the role of diffusivities has been added to the manuscript.

p.8771 This very nice introduction to the complexity of chemistry is surprising in focusing on the hypothetical Brusselator model of Prigogine (which an excellent toy example of chaotic and oscillatory behavior) but not mentioning the real Belousov-Zhabotinsky (BZ) reaction which has similar transient complex oscillations in a batch reactor.

Response: Agreed

Changes to the manuscript: Sentence added in the introduction.

What is missing here is a section on the studies of realistic stratospheric ozone chemistry and how the cascading microscales of mixing are expected to affect reaction rates in non-linear ways. Really nice work includes: Thuburn and Tan (1997 JGR, "A parameterization of mix-down time for atmospheric chemicals") and Tuck et al. (1995 JChemSoc-Faraday, "Airborne chemistry and dynamics at the edge of the 1994 Antarctic vortex"). It is a reminder of what is not included in these toy chemistry tests.

Response: We agree that this is an interesting angle but is too focused to be included in this study.

Changes to the manuscript: None.

p.8772 I remember several studies documenting the lack of conservation of Cl-y and the ensuing problems, but the only one I can find is the Strahan et al. study (2011 JGR, "Using transport diagnostics to understand chemistry climate model ozone simulations"), which pointed out this problem of Cl-y conservations in a non-toy chemistry and its importance: "model Cl chemistry and conservation problems [in 3 models] also have a significant effect on return date." It should be part of the history of why this paper addresses an important problem.

Response: Agreed.

Changes to the manuscript: Strahan reference added.

p.8773 There is a lot of effort to lay out the simple Cl-Cl2 equations and come up with some closed-form analytic solutions. Given the time dependence and mixing a steady-state seems to be not that useful. I was surprised that the time constant of the system was not derived since that is relevant compared to the model time step – from the Jacobian I calculated a time scale of -1/(k1 + 4 k2 [Cl]), which of course depends on the [Cl] abundance.

Response: We acknowledge that the initial condition is secondary as long as the

weighted sum of the species add up to a constant. We also agree that the derivation of the steady-state solution is not essential for the test case but it may be useful for debugging (test chemistry solvers). The Jacobian is listed in the Appendix.

Changes to the manuscript: The derivation has been moved to an Appendix.

p.8774 The equation (9) is technically correct, but why not just tell the reader that the sines and cosines are just the cosine of the solar zenith angle (SZA). This is a toy model that I would not have chosen since it has the photolysis rate falling off as the cos(SZA). For the types of species envisaged here, and the ones causing problems in the upper stratosphere, the photolysis occurs in the visible and is either 'on' or 'off' (dark side of terminator), this soft edge in the rate is much easier to model that the almost Heaviside function. (Although in reality there is a twilight period when photolysis occurs only through scattered light from overhead molecules.

Response: Agreed.

Changes to the manuscript: SZA is explicitly mentioned in the manuscript.

p.8775 I do not see the reason for these derivations, put in SM? It would be better to initialize with a simple [0, 1] set of values for [Cl] and [Cl2] as these are too complex and the system is simply not in steady state so why bother? Start it all as Cl2. Also the variable D get used in (16) and finally defined in (22)? Is this right. Furthermore, 'D' is too close to the differential use in (4-6) of D/Dt.

Response: We compute the steady-state solution to minimize potential shock to the system - we wanted to make sure that the noise we were seeing was not due to chemistry but solely due to transport. We changed capital d in the differentials.

Changes to the manuscript: Derivation moved to the Appendix.

p.8778 This discussion of shape preserving filters being effective flux limiters seems limited (no pun). Other methods also originated shape-preserving approaches to eliminate negatives and ripples and preserve of species correlations. These are described

in the authors' previous paper, Lauritzen et al. (2012 GMD), why not here?

Response: OK

Changes to the manuscript: The following paragraph has been added to section 2:

Typically, transport operators are not applied in their unlimited versions in full models. Shape-preserving filters are applied to ensure physically realizable solutions such as the prevention of negative mixing ratios or unphysical oscillations in the numerical solutions (e.g. Durran, 2010). The filter method/algorithm depends on the advection scheme formulation and discretization. Finite-volume discretizations that are based on cell-average prognostic variables ($\rho\phi$) usually make use of either sub-grid-cell reconstruction function filters, e.g. van Leer type 1-D limiters (Lin et al., 1994), or flux-limiting methods such as flux-corrected transport (Zalesak, 1979). The reconstruction filter can be applied for schemes that are based on Lagrangian or Eulerian finite-volume discretizations, where the integration is based on swept areas (in either dimensionally split 1D operators such as Lin and Rood, 1996, or fully 2D) that span the domain without gaps or overlaps. Examples of reconstruction function filters are Colella and Woodward (1984) and Lin and Rood (1996). Limiting through flux-correction, where low-order shape-preserving fluxes are optimally blended with higher-order fluxes, can only be applied in flux-form schemes. For discretizations based on a non-conservative form (advective form), where the prognostic variables are mixing ratio ϕ rather than $\rho\phi$, tracer mass conservation is not inherent and is usually restored *a posteriori* with *ad hoc* methods (e.g., Priestley, 1993; Gravel and Staniforth, 1994). Since the mass-restoration algorithm may alter ϕ, the mass-fixer and shape-preservation algorithms are intrinsically related. Usually this problem is solved using optimization/variational methods (e.g., White and Dongarra, 2011). For methods where the prognostic variables are represented with series-expansions (e.g., Galerkin methods), shape-preservation can also be enforced with optimization methods (e.g., Guba et al., 2014).

p.8779-80 If you need this detailed discussion it could be made clear. Using the system in CAM-SE is not needed as others will have their own approach to nested loops. The nomenclature of nsplit and ftype is also not logical and presumably a holdover from some ancient coding of CAM. The essence is that we have a time step for "dynamics" (tracer transport) and one for "chemistry" (you can call it physics, but why confuse the reader). These two time steps need not be nested but do need to synchronize at a designated super-time step, e.g., 1 hr = 60 min. Then the transport could be run at a time scale like 12 min that is 'activated' 5 times during the hour. The chemistry operator could have a time step of 10 min and be activated 6 times. The super loop just goes thru minute-by-minute and determines which step is performed. The idea that the transport time step must be a subset of the chemistry one is unnecessary and could prove wasteful. There will be chemistry-transport systems for which chemistry steps must be smaller and others for which the transport step needs to be reduced. GMD readers do not benefit from discussion of the 'namelist', this is not a manual.

Response: Agreed.

Changes to the manuscript: The details of the CAM namelist has been moved to the Appendix. The main text now operates with a transport time-step, chemistry time-step and coupling time-step. Changes have been made throughout the main text (and Figure 6) to accommodate this change in notation.

p.8781/L19 "diving" = dividing?

Changes to the manuscript: Corrected!

Final. The remainder of the paper and the computational results are well presented and very useful. It is worrisome that the l-inf norm has errors >10% in Cl-y conservation. But alas, that is seen in the models diagnosed by Strahan et al. (2011).

Thanks.

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