

Interactive comment on “Quantifying atmospheric transport, chemistry, and mixing using a new trajectory-box model and a global atmospheric-chemistry GCM” by H. Riede et al.

Anonymous Referee #2

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This article describes the simultaneous implementation of a Lagrangian chemical transport model along with an Eulerian chemical transport model and an atmospheric-chemistry GCM. The chemistry modules among each are consistent, allowing for separation of the influence of modeled transport, mixing and chemistry on specific source or receptor regions. These tools are presented and applied to a test case. The overall scope fits with the specifications of a GMC model development paper; however, the article feels a bit pre-mature in some areas. Specifically, the introduction and comparisons to other works is lacking, the paper lacks explanations of some assumptions and conclusions, and the use of vague jargon hinders comprehension. Since the underlying work appears to be technically sound, dealing with these issues will likely only

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require moderate revisions.

Specific comments:

0.0.1 Introduction

- Please present your work in context with regards to existing computational methods used for distinguishing between chemistry, transport and mixing. For example, how does this approach compare to integrated process analysis in CMAQ? To adjoint or DDM sensitivity analysis? To using inert tracers (or simulations with chemistry turned off) to quantify dilution along a given trajectory? This will give you an opportunity to more specifically highlight the benefits of your approach, which at the moment do not entirely come across in the presentation.
- Explanations of previous works are not sufficient. Lines like “All of these models have been designed for their own special purpose” (p457, 15) or “more sophisticated approaches, such as presented in Lehmann (2004) are required (p466, 25)” are very vague. Please expand and consolidate to the introduction. Also include therein the introductory discussion of statistical approach currently presented in Section 3.
- Also consider toning down the “novelty” claims; the use of Lagrangian vs Eulerian models to quantify the effects of mixing is not entirely new. There are text-book examples that touch on this concept in Seinfeld & Pandis. The work of Manomon et al. (2007)¹ also uses 3D fields from an Eulerian CTM to constrain a Lagrangian model. So be careful to distinguish what is being presented as new methods vs new applications of existing methods.

¹ Manomon, R., L. Xiaon and P. Wongwises, A new Lagrangian – Eulerian coupling model system, *Advances in Atmospheric Sciences*, 17(4), 10.1007/s00376-000-0022-9, 2007.

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0.0.2 Writing clarifications

I found many of the statements to be vague and difficult to interpret. Here is a list of places where I strongly encourage to authors to expand on the intended meaning using clear and precise language.

- (numerous places) “quantification analysis”. It took me a while to figure out what you mean by this phrase. Is it: quantifying the contribution of various processes to the chemical concentrations at source or receptor sites? Or shorter: physical and chemical process attributions?
- (p457, 24) “submodels to various base models” Please define the usage of these terms.
- (p458, 24) what is meant by “pure chemistry”? Is there another kind of chemistry?
- (p459, 10) “uncertainty concerning chemistry”. What aspect of uncertainty regarding chemistry are you referring to? Error in rate constants? Missing reactions in the mechanism? Numerical errors? Resolution artifacts?
- (p462, 12) Please clarify what is meant by “individual waypoints” and “requirement for equidistance...”
- (p465, 1) “frayed out” – what does this mean?
- (many places) “dynamic situation.” What does this phrase mean? The local meteorology perhaps?
- (p466, 14) “mixing is only defined within the model hierarchy” – what does this mean?
- (a few places) “keeping its statistical weight”. ?

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- (many places) “transferability... to observations” and “transfer of results” What does this phrase mean? Are you talking about interpreting the trends in observations, or understanding sources, or errors in comparisons between models and observations owing to model resolution...?

0.0.3 Assumptions and explanations

Here is a list of assumptions or results that are stated or claimed, but not supported by any justification or evidence. I’m not saying these are mistakes, just aspects that are not explained clearly or at all.

- (p461) Why is sedimentation and deposition switched off? Was this for computational convenience? If so, why are these complicated to include? If not, was this necessary for theoretical reasons to facilitate interpretation of results, and would it thus be a limitation to applying this technique to any cases with real observations, for which these processes are necessary?
- ...same for aerosol chemistry – why neglected?
- ...same for heterogenous reactions – why neglected?
- .. same for cloud fraction and cloud water content – why set to zero?
- (p466, 23) Why is the chemical analysis only applicable to slow species?
- (p469, 13) “method presented here is a time-efficient tool”. How is efficiency measured? Efficient compared to what? Why is doing the calculations offline efficient?
- (p464, 27) “38,15,9,40” Why the reversal of the trend when going from 9 to 40?