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Geoscientific Model Development Discussions

Interactive comment on "Simplified aerosol modeling for variational data assimilation" *by* N. Huneeus et al.

D. Henze (Referee)

daven.henze@colorado.edu

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Review of "Simplified aerosol modeling for variational data assimilation."

The authors present a new simplified model for global aerosol distributions, with the primary aim being estimates of aerosol optical depth. This simplified model is compared to a more explicit aerosol model as well as with observations. The tangent linear and adjoint versions of the simplified model are presented with examples from each. The technical analysis is mostly sound and the modeling is well done. The presentation could use a bit of work. I have lots of comments, though few that require any additional calculations; they are mainly just clarifications, questions, and suggestions for additional references. Overall, I think this manuscript will be acceptable for

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Discussion Paper

publication in GMD with minor revisions.

0.0.1 Comments

1. abstract: the summary of the comparison between the reduced and full model glosses over some of the differences noted in the manuscript and conclusions. I think space allows for a few more details to be presented regarding the areas and species for which the reduced model is most / least consistent with the full model as well as the observations.

2. introduction: I think it is important to make a greater effort to cover previous modeling developments in this area, not only because of my own contributions in this area, but because the scope of GMD provides a unique platform for focusing on the history of model developments.

   - 641 or 642: It's probably worth mentioning the work of Collins et al. (2001) somewhere, which was one of the first studies to assimilate aerosol optical properties into a CTM.
   - 641.15: Examples of earlier gas-phase variational assimilation works other than those cited in the present manuscript are Marchuk (1974), Robertson and Langner (1998), and Pudykiewicz (1998).
   - 641.18: In discussing the history of variational data assimilation work for aerosols, it should be mentioned that the first adjoint of a detailed, coupled gas and aerosol simulation (GEOS-Chem) was developed by Henze et al., (2007) and applied (Henze et al., 2009) using 4D-Var to estimate emissions of aerosol precursors: NO_x, NH_3 and SO_2.
   - 642.6: "Sandu et al. (2005) developed an aerosol model for inverse modeling of aerosol dynamics that focuses only on the physical particle dynamics excluding the chemical and thermodynamic transformations." → "Henze et

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al. (2004) and Sandu et al. (2005) developed inverse box models of aerosol dynamics that focus on the physical particle dynamics with limited chemical and thermodynamic transformations."

- 641 or 642: I see Viskari's paper in the bibliography, but it is not referenced anywhere. It should probably be included somewhere around here.
- 641 or 642: DDM aerosol models (e.g., Koo et al., 2007; Napelenok et al., 2008) are essentially tangent linear aerosol models, which although not yet used for variational data assimilation, address many of the modeling issues (linearity, model reduction) touched upon in the present article, and are hence probably worth mentioning.

3. general: Why use a simplified model? Is is because of the computational expense of detailed aerosol models may become prohibitive for the scope of your intended data assimilation applications, or because there are aspects of the full model not amenable to automatic differentiation with TAPENADE?

4. 650.10: "Fine mode AOD computations are only conducted over ocean since MODIS retrievals for the fine mode AOD are not reliable over land." Discussion about linearity in the fine mode simulation is limited to only over oceans, but otherwise the rest of the manuscript discusses fine mode simulations throughout the globe. As it should. I don't recommend limiting the applicability of your work to a single satellite product. There are other MODIS products with improved performance over land (eg., Drury et al., 2008) in addition to several other satellites (OMI, PARASOL, CALIOP, someday even GLORY) for which the model presented here is of value.

5. 651.3: I find that people often struggle to understand wether the spatial distribution of values in a plot of sensitivities ($\partial y/\partial x$) represents the spatial distribution of the numerator or denominator. It may help your discussion to rephrase the following sentence "namely maximum sensitivity in AOD to perturbations in the emis-

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sions of desert dust particularly over Central Asia, large sensitivities to emissions of sea salt and fine mode aerosols (species 2)" to "namely maximum sensitivity in AOD over Central Asia to the perturbations." It seems a bit premature at this point to specify which aspect of the perturbations the sensitivities reflect as they reflect the sensitivity with respect to all of the perturbations for all species emissions in all locations as well as the chemical lifetime of the gaseous precursors. While such information can be speculated, that type of analysis is more appropriate for the adjoint sensitivities discussed later. The same potential for confusion arrises when discussing model sensitivities on page 653. Peaks in the TLM sensitivities are attributed to sources. Yet as shown in the adjoint modeling section, the influence of sources can be quite distant. Further, over short time periods the peaks may reflect locations of secondary aerosol production from SO_2 owing to an area of heavy cloud processing rather than a location of a specific source.

6. 651.13: "Sensitivity tests (not shown) . . . ..." I find it odd that this is the only result from your sensitivity analysis that is mentioned in the abstract, yet the actual analysis is not presented. Basically, I would like to see this analysis if it's going to be treated as a primary finding of the paper.

7. section 3.2.2: Some of the analysis in this section may be misleading; a factor of 3 difference between the AOD response to a 10% BB perturbation compared to a 10% FF perturbation might just mean that BB emissions were three times larger than FF emissions during the selected analysis period. To avoid this issue, normalize the sensitivities with respect to the magnitude of the emissions. You could also compare to sensitivity of AOD at other wavelengths if you fully normalized the results, i.e., $(\partial y/\partial x)(x/y)$.

8. 654.24: "Differences in magnitude. . . " This isn't the clearest sentence, so perhaps I misunderstood, but do you mean to say that the sensitivity with respect to emissions increases as one considers emissions on days that are increasingly

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prior to the observation? You are showing only the sensitivity with respect to emissions on specific days, not the total emissions sensitivities integrated from the observation point back to those days, correct? If so, then wouldn't the influence of emissions on a specific day eventually *decrease* as one considers days further back in time than the average lifetime of the aerosols? In other words, if you look at the sensitivity 20 days back, it is probably smaller than the sensitivity 5 days back, which would contradict the sentence in question.

9. 660.4: "As a consequence, several modifications had to be introduced". This strikes me as a perfect opportunity to test the 4D-Var capabilities of your model in a novel way. Why not generate some pseudo observations with the full model and then assimilate these with the simplified model, letting the system adjust parameters of the simplified model in an optimal fashion such that the simplified model best matches the estimates of the full model?

10. general: comparison of full and simplified models: One frequently mentioned drawback to most 4D-Var studies, compared to filtering approaches, is the assumption that the forward model is perfect. Here, as usual, the simplified forward model is not perfect. However, the authors are in the special position of having just quantified the areas in which the model is imperfect, at least with respect to the LMDz model. How will the information gleaned from the comparisons of the SPLA and LMDz models be used to guide a real data assimilation study or to interpret the results of such study? Could the differences noted here be used to construct model error covariance matrices to be used in a weak-constraint 4D-Var framework (e.g., Trémolet, 2006)?

0.0.2 Minor comments and clarifications

- abstract: Suggest the first sentence be rearranged to read "...simplified aerosol optical depth model together with its tangent linear and adjoint versions for the

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ultimate aim of optimizing global aerosol and aerosol precursor emissions using variational data assimilation.

- 641.4: “small” → “smaller”
- 641.11: “optimal initial state” → “optimal state”
- 641.18: “aerosol emissions” →“aerosol and/or aerosol precursor emissions”
- 644.23: “The conversion from terpenes to OC varies from 0.1 to 15%”. Actually, the SOA mass yields for some terpenes can be greater than 100% (e.g., Ng et al., 2007), so it might be prudent to revise this statement.
- 647.6: Do you really mean POM (an acronym not yet defined but likely meaning primary organic matter)? If so, what happened to the secondary organic aerosol from terpene oxidation? Please check usage of POM on page 656 as well.
- 650.16: “This can be obtained . . . ” Can this sentence be expanded and clarified?
- 650.21: “compare it with the difference . . . ”. This is a bit vague. I think it would be clearer to write out in equations the comparison that is being made here: $H(\mathbf{x}) - H(\mathbf{x}+\delta\mathbf{x}) = \mathbf{H}\delta\mathbf{x}$ + *nonlinear terms*. Also, any error in construction of **H** might accidentally get lumped into the nonlinear terms. So it would be nice to mention, as you do for the adjoint model, that **H** has been numerically validated.
- throughout: should differentiate between scalars and vectors using bold.
- 651.17: “July 2002 are shown.” → ”July, 2002.”
- 651.21: I don’t think the BB and FF acronyms have been defined.
- 654.4: “130 times” excellent! Any comment on the computation expense relative to the forward model, or the size of the checkpoint files relative to the model grid size and time step?

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- 642.20: similar to the flow presented in the conclusions, I think it would be better to place the contents of section 4 directly after introduction of the reduced model (3.1) and before the sections on sensitivity analysis. So make section 3 all about the definition and validation of the reduced model, and then make what are currently sections 3.2 and 3.4 into section 4.
- conclusions: “Variational data assimilation techniques have been developed for individual aerosol species that determine the emissions field that represents the best compromise between a given set of observations and the *a priori* information.” While that is the ultimate goal, only some of the tools necessary for performing variational data assimilation have been presented thus far. Other components, such as the optimization algorithm and construction of *a priori* and observation error covariance matrices, have yet to be addressed.

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