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Geoscientific Model Development Discussions

Interactive comment on "Development of 3D Variational Assimilation System Based on GRAPES-CUACE Adjoint Model (GRAPES-CUACE-3D-Var V1.0) and Its Application in Emission Inversion" *by* Chao Wang et al.

Anonymous Referee #2

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This manuscript presents a new chemical data assimilation system. While the work seems well motivated and potentially valuable eventually, overall the effort comes across as the first step in what needs to be a more thorough study prior to publication. From the onset, the manuscript struggles to explain why they are using an adjoint model for 3D-Var (typically this would be used for 4D-Var), which is then confused as they proceed to describe what is essentially a 4D-Var system but then provide code for something that seems like 3D-Var. . .. it become very unclear what is the scope and objective. Further, the authors neglect to treat prior information in a Bayesian manner,

leading to an ad hoc approach that is not justified. Other issues such as a lack of an appropriate dataset for testing, lack of cross validation, no exploration of the role of prior error covariances, and also the unavailability of the underlying model code amount to this work seeming rather premature. I look forward to a complete manuscript being submitted at a later date, here or elsewhere.

Main comments:

The introduction briefly mentions many previous 4D-Var studies that have used adjoint models for estimating emissions of aerosols and trace gases. However, it is not discussed anywhere why the authors are using their adjoint model for 3D, what is the background of other studies using 3D-Var, and how this compares to 4D-Var. Nor is very much background provided about the GRAPES-CUACE model âĂŤ it isn't even mentioned until the final paragraph. No background on model performance is discussed that motivates the need for the GRAPES-CUACE 3D-Var. In other words, the introduction is not written very specifically for this manuscript.

Section 2.1: Given this is a paper in GMD, the description of the model needs to be much more complete. Here is a brief list of immediate questions; the authors would need to revise to address these and also provide a more detailed and complete description of the model in general.

What gas phase species are included? Does the model account for gas phase oxidation SO2 to SO4, or NOx to HNO3? Several recent papers have shown that NH3 plays an important role in governing aerosol concentrations in this region, given its role ammonium nitrate. However, it appears this model does not include NH3 or NH4, is that correct? How is missing this key species going to impact the results of this model? Another significant component of urban PM2.5 in the BTH region is secondary organic aerosol (SOA). Is any SOA included in this model, or is all the organic carbon assumed to be primary? If not, how does this bias the resulting calculations? How do the authors convert from mass of organic carbon to total mass for estimating PM2.5? Is the PM2.5

concentration estimated at dry or wet (i.e. including H2O in the mass) conditions, and if so, at what RH?

There should be discussion of model evaluation, ie comparison against in situ measurements, either here or elsewhere.

134-138: This sounds like 4D-Var, unless the GRAPES-CUACES model itself is only 2D. Can the authors please clarify why they describe their system as 3D-Var?

140-142: Being “classic” or “simple” isn’t necessarily a good thing. In this case, the steepest decent method can be highly inefficient, requiring many more iterations to reach the minimum than other approaches. Given the wide availability of more advanced gradient-based minimization algorithms (such as quasi-newton variable metric methods like L-BGFS-B), it’s not clear why the authors chose the steepest descent method.

Section 2.5: Here is where the authors should describe in detail the following highly critical components of the inversion: gamma, B and R. What are their values? What assumptions were made in comping up with those values? What simulation experiments were considered to evaluate how robust the model inversion performance is for these values? etc.

Section 2.6: Here the authors provide a few sentences about the data that is missing (ie, measurements of BC), but they provide very little information about the data that is actually used. Instead, they need to describe the measurements used in this study, addressing the following points: how many cites? where are they located (provide figure)? what species do they measure? at what RH are the masses recorded? what is the frequency of the observations? what instruments are used to make the measurements?

190-200: So the inversion is only performed for this brief period of a few days? While a good place to start, this seems very preliminary and only the first step of a study that

needs to be completed prior to being published.

197: It is not clear to me what the authors mean by “inversion area” âĂŤ is this the only region over which they are optimizing the emissions? Why would they artificially define such a region? The adjoint model should give them gradients with respect to each emission within their model domain, and any emission with a significant gradient should be optimized. Only adjusting emission in a pre-defined region will bias the results by over-adjusting these emissions.

205: Two major problems here: (1) Scientifically, this is a very bad idea; source inversion problems are ill-posed. The authors need to include some sort of prior constraint / regularization. The paper is recommended for rejection based on this alone. Note that if the penalty term is removed and R is assumed to be a uniform diagonal matrix, R itself has little to no impact on the inversion, which is also not good. Well formulated inversions are critically dependent upon R and B âĂŤ this needs to be taken further into account.

(2) In terms of manuscript presentation, the authors have already defined the cost function, in a different form, using different notation âĂŤ they need to introduce one and only one set of notation and definition for the the cost function in section 2, and then use that in section 3. Introducing one but using another is confusing.

220 - 225: This interpretation is not correct. For a multiplicative relation ship of a*b*10, one can not ascribe the factor of 10 as being related to b any more than a, since both a*(b*10) and (a*10)*b are equivalent. The introduction of these subjective rescaling of 10 or 100 is arbitrary and likely just compensation for some other deficiency in the inversion framework. The Bayesian approach for including prior information in the inversion via equation 6 is the best way to incorporate the prior into the inversion framework; the authors should stick with that approach.

4.3: The authors use a comparison of the posterior model to the observations used during the inversion as a means of validation. This is a rather weak test, as by definition

if the cost function has reduced, then the model is going to do a better job of matching these observations. Instead, the authors should test against an independent set of observations (not used during the inversion), or consider methods for calculating the posterior error in the emissions themselves (comparison to other studies, estimation using numerical techniques from the inversion, etc).

Code: I checked both web sites provided for downloading the GRAPES-CUACE model and did not see code download at either location. The urls provided are generic links for large institutions. This does not meet the minimum standard of code availability for GMD.

I also reviewed the code provided the supplemental. I do not see how this code accomplishes the steps described in the paper. I don't see where the information for the adjoint is input into the optimization routine, where the updated scaling factors are calculated, and where these are provided to the forward model to run, iteratively. The optimization seems to be running entirely offline, which would be consistent with 3D-Var; however the process described the manuscript and the accompanying flow chart (fig 3) shows a 4D-Var system. In general, the code is not well documented nor explained, which again is antithetical to the purpose of publishing in GMD. It also appears to allow for the cost function to have "converged" if it is increasing, rather than decreasing, which is odd. Shouldn't J(k+2) always be less than J(k+1)?

- The grammar and writing needs a lot of work throughout, pretty much every sentence. It goes beyond my responsibility to edit in this detail, but the authors will need to hire editing services or engage additional co-authors to help with this in their next submissions.

Other:

Throughout: Use the phrase a priori / a posteriori OR prior / posterior consistently throughout, and do not mix-and-match.

23 - 25: rewrite, not clear

42: What is meant by "reverse optimization"?

82: I don't think the nationality of the people who developed the model is scientifically relevant.

128: Can the authors be more specific here? What was checked, and how accurate did they find the performance to be?

150: It is more correct to say that the cost function is based on the Bayesian method. The adjoint is just a tool used for finding the minimum of this cost function. Strictly speaking, there is no such thing as an "adjoint inversion", since the adjoint is just one piece of the overall inversion framework. I know that people may say that, casually, but in scientific manuscripts we should be more careful. Bayesian method leads to the cost function. One approach to minimizing the cost function is 4D-Var. An adjoint is just a part of the numerical tools we often use as part of 4D-Var (keep in mind it is possible to do 4D-Var without an adjoint. . .).

161: Technically FˆT is the transpose of the model Jacobian. In contrast, the adjoint model is what is used to solve the product of FˆT and a vector. The vector here would be the adjoint forcing, Rˆ(-1)(H(x) - y)

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