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Atmospheric Chemistry and Physics
Discussions

Interactive comment on "Global sensitivity analysis of GEOS-Chem modeled ozone and hydrogen oxides during the INTEX campaigns" *by* Kenneth E. Christian et al.

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We thank the referee for their thorough review and thoughtful suggestions for improving the manuscript. Below are our responses to the referee's comments (*italics*).

1 General comments

This manuscript presents a global uncertainty analysis of the concentration of oxidants (O_3, OH, and HO_2) at various altitudes through the troposphere, and in four geographical regions (central and northeastern U.S. and Canada, Gulf of Mexico, Pacific ocean near Honolulu, Hawaii, and Pacific ocean near the southern coast of Alaska). The

authors use an ensemble of 512 GEOS-Chem simulations in which various inputs have been pseudo-randomly perturbed within prescribed uncertainty ranges, along with the high dimensional model representation (HDMR) technique to apportion the uncertainty in modeled oxidant concentrations to each of the perturbed inputs. The geographical regions studied in the manuscript feature various chemical and meteorological regimes and different local and upwind emissions profiles. Comparison of the results for these regions brings valuable insight into the model inputs that influence oxidant concentrations in these various conditions. The study is well conducted and the results are clearly presented and explained. A concern for the publication of this manuscript is the similarity of this study with a previous study (Christian et al., 2017a), mostly by the same authors. I do think that the proposed manuscript brings significant new contributions that warrant publication, but the authors should discuss more explicitly the insights that are novel and significant in this manuscript compared to the authors' previous work. The sections below describe in more detail the suggestions and comments that I would ask the authors to address prior to publication.

2 Specific comments

As mentioned in the Overview section, the authors should discuss the novel insights that this study brings compared to the previous work of Christian et al. (2017a). One novel and insightful aspect of the proposed manuscript seems to be the comparison of the uncertainty apportionment between different regions, as well as the vertical resolution of the analysis.

Response: Compared to our previous study, there aren't too many differences in the methodology to highlight. As noted, we have presented the results in a slightly different format compared to the ARCTAS study with the sensitivities split vertically but this is more to highlight the vertically variable nature of these values. Perhaps the biggest difference between this study and the last is the inclusion of box model profiles for further comparison to the global model and measurements. Clearly the domains in this study are very different than the remote Arctic. These North American and remote maritime domains are affected by a different set of local emissions and different chemical regimes.

Changes: Changed sentence to make note of difference between Christian et al., 2017a and this study (P6 L25).

A similarly worded description of HDMR is already present in the previous work. Although it is useful for the proposed manuscript to summarize the principal concepts of this method, I suggest this description be re-worded further. The same comment applies to other parts of the "Methods" section.

Response: We have expanded a bit on our methods section and the description of the HDMR method. Much of this is covered in our response to your later suggestions.

Page 4, Equation (1): shouldn't $f_i(x_j)$ be $f_i(x_i)$ instead?

Response: Yes, Changed as suggested. P4 Equation 1.

Page 2, Lines 16-22: "Instead, the sensitivity analyses of GEOS-Chem modeled results has either used local methods in which the factor of interest is perturbed individually and compared to the model state without this perturbation, or the GEOS-Chem adjoint (Henze et al., 2007). [...] While useful in determining some individual sensitivities, these methods neither can nor were intentioned to provide a complete picture of model sensitivities in which many inputs have uncertainties." The adjoint sensitivity technique can be used to efficiently calculate first-order sensitivities of a model metric or cost function to many model inputs (sensitivities of a given model

metric or cost function to all model inputs can be efficiently calculated with a single "adjoint simulation"). Although the results from such an analysis provide "only" first-order local sensitivities, one can argue that they do provide a fairly comprehensive picture of model sensitivities for a given metric and a large number of model inputs that have uncertainties. A strength of the HDMR method used in the proposed manuscript resides in the fact that model non-linearities are accounted for in the propagation of uncertainties, while other sensitivity approaches are often limited to first-order sensitivities. However, the HDMR approach does require a large number of model simulations (512 here). Additionally, the apportionment of the overall uncertainty with the HDRM method relies on a priori estimates of the uncertainties on relevant inputs. Sensitivity or uncertainty apportionments based on other sensitivity methods often do not depend on such a priori estimates. Could the authors discuss these considerations in greater detail in the manuscript prior to publication?

Response: It is a good idea to expand a bit on the strengths and weaknesses of this method in the context of the other sensitivity/uncertainty analysis methods currently used in the community. There are strengths and weaknesses in both the HDMR method and adjoint methods and there is quite a bit of overlap between the applications of adjoint and HDMR sensitivity tests, but there are some differences worth highlighting. For one, while adjoint models can be used to calculate model sensitivities, they are not necessarily used to determine the model uncertainty. Where the HDMR calculates the portion of the total model uncertainty attributable to the uncertainties in different factors, adjoint sensitivity tests do not put their sensitivities into the context of the total model uncertainty and do not fully sample the input space beyond some small perturbations. Secondly, the adjoint sensitivity tests can only be used for one output or cost function per test. In our cases we were looking at model-measurement agreement for multiple time periods during the field campaigns and for multiple outputs along these flight tracks. With our ensemble of model runs completed, we can easily compute sensitivities for any of a variety of different model outputs for any subset of the field campaigns with negligible additional computational cost. Considering the differences in calculating adjoint sensitivities and the sensitivities calculated by the HDMR method, we hope that these results will be complementary to the work being done in the inverse modeling and adjoint community. We have reworded the introduction to make note of the work being done in the adjoint community and note the strengths and weaknesses of this method in comparison to the adjoint method.

Changes: Reworded third paragraph to mention and compare these methods to the adjoint sensitivity work. P2 L13-28

Page 3, Lines 18–20: "As uncertainties are not published for the meteorological models, we define our meteorological uncertainties as the average of the monthly standard deviations of the difference between GEOS-4 and GEOS-5 meteorological fields for 2005, a year of overlap between the models." How different are these two models? If they are fairly similar, the uncertainties on meteorological inputs may be significantly underestimated. Can the authors discuss the fairness of this assumption?

Response: The two models are more similar than dissimilar, but there are many differences between the two:
The native resolutions are different between the models (1x1.25 for GEOS-4, 0.5x0.666 for GEOS-5)
The data assimilation techniques used are different
The convective parameterizations are different
Cloud fraction and optical depth can be very different
http://wiki.seas.harvard.edu/geos-chem/index.php/Overview_of_GMAO_met_data_products#GEOS-4

With some back of the envelope calculations, we find similar uncertainties when

comparing the flight track temperatures between the model and measurements (~2K vs 1.8K). Winds and some of the other meteorological factors perturbed in this study weren't measured on the aircraft. While our defining the uncertainties by the difference between models may result in some underpredictions, we are likely fairly close.

Page 3, Lines 12-13: "In general, there were typically small differences between modeled results using either 4 x 5 or 2 x 2.5 resolutions but we illustrate in our results where this is not the case." The authors do discuss some of these differences in the Results section (for example: section 3.1.2), but it would be insightful to see more quantitative information describing the model-versus-observationss agreement (for example: mean bias, standard deviation) with the lower resolution simulations on the one-hand, compared to the higher resolution simulations on the other hand.

Response: We did not discuss the differences between the coarse and fine results outside of the Houston flights because the differences were quite small compared to the differences seen among the different perturbed model runs. For those interested in the differences between these resolutions we have added a comparison of the two resolutions for each domain and added the fine resolution profiles to the supplement.

Changes: Added/expanded discussion of fine vs. coarse model resolution for each domain. P8 L5-7; P8 L19-23; P9 L6-8; P9 L27-20 and fine vs. coarse profiles to the supplement.

Page 5, Equations (3) and (4): I am unsure as to whether ${\varphi^i}_r$ in equation (3) is the same as ${\varphi^i}_p$ and ${\varphi^j}_q$ in equation (4) if r = p = q and i = j. Additionally, the use of superscripts as indices can also introduce confusion. Can the authors add text to clarify these concepts?

Response: We have added more descriptions of the what all the indices mean in the Methods section and added citations to direct readers to the papers that cover how some of these functions are created. The superscripts as indices follows convention established in previous HDMR papers. To lessen this confusion we have added some additional text to describe what these constants mean and removed the equation describing the calculation of the second order polynomials since we don't discuss these indices specifically anyways.

Changes: Various changes to the equations and their descriptions (P5).

Can the authors discuss the contributions of uncertainties associated with inputs interacting with one another (i.e. "missing" slices in Figures 6–9), and the significance of these missing slices for the interpretation of the results presented in the manuscript?

Response: The "missing" portion of the pie charts represent the portion of the total variance not accounted for by the variances of the first order sensitivity indices. One can think of this as some of the "non-linear" interactions between factors. While the software calculates these polynomials representing the co-varying of two factors at a time, we are not as confident in these values. Also these sensitivity indices are individually smaller than the first order indices. We are confident in our first order indices as we have tested the sensitivity indices calculated with varying numbers of model runs and find the sensitivity indices to converge upon a consistent value after 256 runs or so giving us confidence in the first order sensitivity indices presented here. (See Reviewer 1 Comment 1).

Changes: Made note of the missing portion of the pies on P10 L11-13

3 Technical corrections: The authors repeatedly use the word "standard" to refer to notions such as "common practice" or "default value" or "default configuration". I suggest that the word "standard" be reserved for a more restrictive meaning of the word (i.e. a formalized norm or convention). Examples:
Page 3, Line 8: "We use in this study the standard GEOS-Chem model"
Page 3, Line 21: "the model ensemble made use of the standard emissions inventories"
Page 4, Line 7: "the standard model treatment"
Page 14, Line 21: "as opposed to the standard 0.20"
In what follows, text that I suggest be removed is written inside curly braces and in red, and suggested replacement text is in blue. Page 2, Line 15: "save for {a} some recent work"

Changed as suggested

Page 3, Line 8: "We use in this study the standard GEOS-Chem model (v9-02), a {popular} widely-used global chemical transport model"
Page 3, Line 21: "{For much of the developed world} For many industrialized regions"
Page 6, line 29: "During INTEX-A, the NASA DC-8 primarily sampled the eastern half of the United States and Canada {INTEX-A} during the summer of 2004"
Page 9, Line 5-6: "aerosol uptake {to} of HO_2"
Page 9, Lines 8-9: "In contrast, {uncertainty} uncertainties in both OH and HO_2 mixing ratios were considerable"
Figures 6-9: the different colors used in these Figures translate to very similar shades of gray when converted to gray-scale. I suggest changing some of these colors so that the different categories of inputs (Emissions, Kinetics, Photolysis, Meteorology, Heterogeneous) can be more easily distinguished when these Figures are converted

to gray-scale. I also suggest showing on these Figures the numerical values corresponding to the slices (i.e. contribution of each input to total uncertainty, in %), at least for the largest slices.

Response and Changes: The colors were chosen using the ColorBrewer tool to optimize color viewing. To add some contrast, we have changed the colors of a couple of the categories. We have also taken the suggestion to add the sensitivity indices to the larger portions of the pie (any slice > 0.10).

Acknowledgments: "University Maryland". Missing word "of"?

Response: Correct. We thank the reviewer for finding this typo.

Changes: Changed as suggested (P15 L31)

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