**Atmospheric
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Discussions**

Interactive
Comment

Interactive comment on "Parametric sensitivity and uncertainty analysis of dimethylsulfide oxidation in the remote marine boundary layer" *by* D. D. Lucas and R. G. Prinn

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Comment 1: "The sensitivity analysis run in this paper is somehow old fashioned, in what it misses much of the recent methodological work on the topic... In particular, after having clearly demonstrated that the model is rich in structure and interactions, the authors fail to provide any of the summary measure that would assess the global importance of factors. Take for instance figure 6. It is instructive, but it only maps the total sensitivity of a factor against itself. Where is the effect of the other factors? And where is the synthesis of all that as a measure of ranking the input factors?"

General Reply to Comment 1: We would first like to point out that the meaning of the

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term 'sensitivity' often differs throughout the literature. In our original ACPD paper, we defined 'sensitivity' as the influence of an input at a local point on an output, irrespective of uncertainties. These sensitivities are therefore 'local sensitivities'. We have greatly clarified this in the revised manuscript by changing 'sensitivity' to 'local sensitivity' every place where only local parameter values are considered.

In addition to local sensitivities, our manuscript also calculates the influence of an uncertain input at many points on an uncertain output. These are often known as 'global sensitivities', but our original ACPD paper labeled these as 'uncertainties' and 'variance contributions'. Again, we have greatly clarified this in the revised manuscript by using 'global sensitivity and uncertainty analysis' in the sections that consider the uncertainties of the parameters.

Specific Replies to Comment 1: The DIM-based sensitivities (Eqs. 3 and 6 in the revision) are of the local variety, and their analysis has indeed a long history (old-fashioned in the reviewer's terminology). As a signal to the reader about this, we cite an article from 1976 when we first describe the DIM method at the beginning of Section 3.1 in the revision. The text has also been modified to make it even more clear that this local method is an old, but well-tested, standard method.

Our PCM-based sensitivities (Eqs. 10 and 11 in the revision) are also local, but do serve as a legitimate bridge to global sensitivities because they are easily calculated at many points in the input uncertainty space. Fig. 6 in the original paper displays these only as variations against a single input because the PCM expressions are multi-dimensional (i.e. difficult to plot any other way) and because we only wish to illustrate the large changes in the local sensitivities across the input uncertainty spaces.

In the revised manuscript, we now use Fig. 7 (previously Fig. 6) to emphasize that DIM is not appropriate for the global sensitivity and uncertainty analysis. The revised text in Sections 3.2.2 and 4.2.3 solidifies these points. Also, we now highlight Fig. 10 in the revision as the place where readers should look for drawing important conclusions

about the effects of uncertain inputs on uncertain outputs.

Lastly, though this may have been lost in the original text, we actually do provide a synthesis measure that assesses the global importance of factors (see also our response to comment 6 below). This measure covers the full uncertainty space of all parameters, includes the effects of other factors (including parameter interactions), and provides a quantitative ranking of the input factors. This measure is calculated by taking the expected values of the polynomial chaos expansions (see Eq. 15). The revised Section 3.2 better describes the global analysis and the resulting quantitative ranking using PCM in Fig. 10 is stressed even more.

Comment 2: "The authors have estimated their model over a large set of Monte Carlo runs. Could they produce the model coefficient of determination for the set as a function of time for selected output variables? A suggestion would also be to compute on these the input - output standardised regression coefficients, a measure that provides for multidimensional averaging (the effect of X(I) on Y(K) is averaged over the space of X(I) as well as over the space of all X(J), J different from I."

Reply to Comment 2: Our main purpose for the brute-force Monte Carlo is to provide a basis for comparing between the true model and PCM-based approximations of the model (Eqs. 1 and 9 in the revision). After determining that the PCM approximations are adequate, our remaining analysis focuses on using the approximations.

We determine that the approximations are sufficient by calculating the coefficients of determination (R^2) between the outputs of the true model and the approximations. These R^2 are displayed in Fig. 4 in the revision at night (04:00 LT) and midday (12:00 LT). Although the R^2 values vary between night and day, these variations are not very large. We consequently believe that it would not be useful or informative to show the R^2 at other times.

We also note that the coefficients of the PCEs computed by PCM are analogous to the standardized regression coefficients (SRCs). That is, they are determined by fit-

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ting the output of the real model to an expansion of normalized model inputs. Like SRCs, the squares of the PCE coefficients are also directly related to the input-based contributions to the total output variance as explained in Tatang et al. (see Eq. 16 in revision).

Comment 3: "The are a variety of decomposition used for model representations, such as projection pursuits, radial functions, ANOVA high dimension model representation (ANOVAHDMR, often used in sensitivity analysis) and cut-HDMR, often used in SA for chemical systems (Saltelli et al., 2000, a multi author book, covers most of this material. Alternatively see Rabitz et al., 1997). The present paper presents a rather novel representation (from the 1997 paper from Tatang et al.).. The reader might be interested in a mention of the specificity (advantage disadvantage) of this method versus others."

Reply to Comment 3: We are confident that the PCM approach is appropriate and adequate for the chemistry-related goals of our paper. We have not applied the other decomposition techniques, so we feel that we do not have the expertise to ascertain the strengths and weaknesses of each relative to PCM. We have, instead, now cited your book as a source to the other techniques so that the interested reader can find the resources to make such a comparison. This would be an interesting study, but it would be addressing different goals than we have here.

Comment 4: "The author make clearly the point of the inability of the local methods to estimate moment (section 6.3.2). PCM and DIM-M agree with one another, which is good given the resources spent in building PCM, but DIM-S cannot give the same result. Yet in the rest of the paper the authors try to make the point that after all DIM-S sensitivities and DIM-M give the same message. Looking at the results, I would rather say the opposite. If the system were linear, which we agreed it is not, DIM-M should be proportional to dY/dX(I) times sigma(X(I))/sigma(Y), and there is no way that the result can be independent from sigma(X(I)). Furthermore the system is non linear and hence dY/dX changes both with X(I) and with X(<I) (the complementary set)."

Reply to Comment 4: We greatly appreciate this comment on our inconsistency in using the local DIM sensitivities to estimate global uncertainties. We have, accordingly, removed all of the uncertainty estimates using DIM sensitivities, including the temperature-dependent uncertainties towards the end of the paper. We use Figs. 7 and 8 in the revision to justify the removal of these sections. These figures show that the $\partial\eta/\partial\varrho$ vary greatly in the uncertainty space of ϱ and that higher-order sensitivities are important, and so using the local DIM sensitivities as a basis for extrapolating uncertainties (Eq. 7 in the revision) can lead to large errors.

Comment 5: "End of page 10 the importance of CH3SO2 dissociation in Saltelli and Hjorth 1995 versus the present paper. It is only natural that the results using different models differ, yet this conclusion should not be arrived at by comparing local derivatives output with global measures output."

Reply to Comment 5: We thank Dr. Saltelli for pointing out our mistake in comparing the local and global sensitivity results for CH_3SO_2 dissociation. As shown in Fig. 10 in the revision, though, this conclusion still holds for our global analysis. We have therefore moved this comment to Section 4.3.2 in the revised manuscript.

Comment 6: "At the bottomline I would like the authors to try at least a global sensitivity analysis measure, such as e.g. the Morris method (Morris 1991) or other."

Reply to Comment 6: As we understand, global sensitivity analyses rank or quantify the contributions of the uncertain inputs to the uncertain outputs while accounting for the uncertainty spaces of the inputs. The Morris method, for example, estimates the global sensitivity as an average of many local sensitivities calculated at different places in the uncertainty space of the inputs. That said, we argue that the probabilistic collocation method in fact meets the criteria of a global measure and that we have already carried out a global analysis.

There are two clear places to see the global nature of PCM. First, the coefficients of the polynomial chaos expansions (Eq. 9 in revision) are themselves derived by

evaluating the model using different sets of model inputs generated from the PDFs of these inputs (i.e., not just at the parameter means). Second, the PCM-based variances (Eq. 15 in revision) are derived by integrating the representation of the model (i.e., the PCEs) across the full probabilistic space (Eq. 13 in revision) of all the parameters simultaneously (i.e., from the definition of the expected value).

In the revised manuscript, the results of this global analysis from PCM are summarized in Section 4.3 and displayed in Fig. 10. So as to avoid confusion for future readers, we have greatly revised the text to draw a clearer disctinction between our local and global results.

Interactive comment on Atmos. Chem. Phys. Discuss., 4, 6379, 2004.

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