Atmos. Chem. Phys. Discuss., 11, C11687–C11691, 2011
www.atmos-chem-phys-discuss.net/11/C11687/2011/

Atmospheric Chemistry and Physics Discussions

Interactive comment on "Emulation of a complex global aerosol model to quantify sensitivity to uncertain parameters" *by* L. A. Lee et al.

L. A. Lee et al.

l.a.lee@leeds.ac.uk

Received and published: 9 November 2011

The authors wish to thank the reviewer for reading our manuscript and providing an interesting and detailed review. We have replied to the comments below where the comments are made in Italics.

In terms of the types of conclusions this paper attempts to make (e.g. ranking what parameters have the largest impact on the model predicted CCN and the role of interaction effects), the analysis seems quite limited by the capabilities of the software being applied. A monthly averaged model value (from a single month) from two grid cells does not seem sufficient for prioritizing research for a global model of complex aerosol processes (one of the ultimate goals for research of this type that the authors mention in the abstract). It would be very valuable if the software could be extended

to allow for multivariate emulation of the function output as suggested by J. Rougier's ACPD comment in order to build confidence in robustness of the stated conclusions.

We agree that our analysis of two locations (with >20 grid cells through the troposphere) needs to be extended to provide more useful information. However, we believe the information generated for just two locations is new and interesting. This is the first time that an error bar has been put on modelled CCN, including the fractional contributions of each parameter to the total variance, and the altitude dependence of both. This step should not be overlooked in the inevitable desire to generate the entire global picture. Since submission of the paper the authors have found other emulation software that is more easily adaptable to emulation over many grid boxes, and this is currently being applied to produce global maps based on emulating each grid box independently. So far, this work lends confidence to the conclusions made in this paper. A future effort will be to see if multivariate emulation could be used to take account of the extra structure when neighbouring grid boxes are not assumed independent.

The issue of calibration through comparison to observations also seems extremely important. The authors state it is possible to use calibration against observations to remove implausible regions of input space, but in practice this would seem a rather daunting task due to limitations in available observations and the complexity of the modeling system. I wonder if the authors could comment on how difficult these types of extensions really are. Are these very reasonable next steps or is this something that is a long way from being possible for a computer model of this scale and complexity?

This is a very good comment. The issue of calibration is indeed a complex one. The current practice seems to be to tune parameters in global models without taking into account any uncertainty in the model, which we think can result in over-tuning to the data. The calibration that is suggested here is discussed in detail in Kennedy and O'Hagan (2001) and is thought to be an improvement on the current methods because the uncertainties in the model are accounted for and over-tuning is avoided. Another school of thought is reification discussed in Goldstein and Rougier (2007). Although

the improvements to calibration efforts are well-established, the application of these methods to global models is still in its infancy and so to apply these methods here will be an exciting development. The author's first plan is to history match the emulator to available observations by discounting the implausible parameter space thereby reducing the uncertainty in the parameters and recalculating model sensitivities. The authors see this as a reasonable next step. This could be applied across models and is within the scope of the project to quantify the model sensitivity to uncertain parameters. The next, more difficult, step is to include a discrepancy term and rebuild an emulator with the reduced parameter uncertainty space and comparing again to the observations to find the best parameter set taking into account the uncertainties. This would be a major advance in the application of such methods to global models but at present is beyond the scope of the project.

My second question is the justification given that the errors in emulator are sufficiently small and can be completely ignored in the sensitivity analysis. On pages 20451 and 20452 you provide the emulator standard deviation for the CCN concentration at the surface for London (2.1 cm^3) and the remote marine site (.5 cm^3). It is true that these values are quite small compared to the estimated uncertainty due to the input ranges of the 8 sensitivity parameters. However I wonder if this is the most appropriate comparison. Figure 5 shows the 95% confidence intervals for these sites compared to the validation runs. Many of these intervals appear to have standard deviations on the order of 20 cm^3 for the London cell and 5 cm^3 for the remote cell (estimating one quarter the length of the 95% interval). Since you use the emulator to make predictions under these different parameter settings, not just for the base-line conditions, it would seem the error represented by the spread of these confidence intervals is very relevant to the interpretation of your sensitivity analysis. It would be helpful if this issue could be discussed and justified further in the text (or clarified, if I have simply misinterpreted these figures and the conclusions on these pages).

To clarify for London, the emulator uncertainty of 2.1cm^3 is the uncertainty around the

emulator estimate of CCN concentration. In terms of the formula introduced in the Appendix we have $E^*(E(Y)) = 647cm^3$ and $V^*(E(Y)) = 2.1cm^3$. This means that we can accurately estimate CCN taking into account the uncertainty in the prediction of all unknown points such as those in Figure 5. Each estimate of CCN in Figure 5 is obtained from Equation A4 for each parameter set in the validation design, with corresponding uncertainty $\hat{\sigma}^2 c^*(x, x)$ (Equation A5). From Equation A5, $\hat{\sigma}^2 c^*(x, x)$ is approximately 20cm^3. The emulator uncertainty of 2.1cm^3 is then calculated by integrating Equation A5 over the joint distribution of all the uncertain parameters. The expected uncertainty due to the unknown parameters is 106cm^3, denoted $E^*(V(Y))$, with uncertainty $V^*(V(Y))$, which is not calculated. The sensitivities are calculated by partitioning $E^*(V(Y))$ into its various sources, for example $E^*(V(Y|X1))$ but we don't calculate the uncertainty in this value $V^*(V(Y|X1))$ since the calculations are non-trivial and would be computationally costly to calculate compared to the efficiency gained by emulating in the first place. Instead we rely on the fact that the emulator can predict the GLOMAP output within 95% confidence limits. $E^*(V(Y))$ is large compared to, and therefore distinguishable from, $V^*(E(Y))$. The details of how the posterior equations A4 and A5 are used to calculate the sensitivities can be found in Oakley and O'Hagan (2004). We also use plots such as those in Figure 8 to show that the relationships between the estimated CCN and the uncertain parameter is clear compared to the uncertainty in the estimated CCN at each uncertain value. It is clear in Figure 8 that more accurate prediction of the CCN at each value would produce similar relationships and hence similar sensitivities. When the sensitivity is very low it is indistinguishable from the uncertainty in the predicted CCN but we are not interested in these low sensitivity parameters. Together all the plots lend confidence to our stated sensitivities without the need to explicitly calculate the uncertainty. In light of this Line 19, Page 20451 has been slightly amended:

"The small emulator standard deviation here along with the successful validation in Figure 5a shows that using the emulator has had a very small effect on the accuracy with which the parameter sensitivities are estimated and hence we

have an accurate emulator."

One general editorial comment: There are numerous missing commas throughout the entire manuscript (too many to enumerate here). I recommend a technical edit before final submission. A few specific comments for each section.

Done. Changed as specified.

Interactive comment on Atmos. Chem. Phys. Discuss., 11, 20433, 2011.