

Interactive comment on “Advanced methods for uncertainty assessment and global sensitivity analysis of a Eulerian atmospheric chemistry transport model” by K. Aleksankina et al.

Anonymous Referee #1

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General Comments

The authors have made a commendable effort to apply uncertainty and sensitivity analysis methods which have a long theoretical history in the stats literature but have only in recent years begun to be applied to complex models such as this.

Given that they only look at sensitivity to emissions, and conclude that the model is not particularly sensitive to those inputs, it is perhaps a shame that they didn't attempt to include more input variables into the analysis, as there have been a number of published studies which demonstrate that these methods can be used with significantly larger numbers of inputs.

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There are a few concerns regarding the implementation of the methods and the effect that this may have on the validity of the results. In particular please see the points below concerning sample size and emulator validation, which should be addressed before the paper is recommended for publication.

Specific Comments

P5,L2 How many emissions inputs does the model have, and why were the ones used chosen?

P5,L5 Why were the shipping emissions not split by pollutant type when the other emissions were? Does this not make the results harder to interpret?

P6,L19 Could the authors include their reasoning for choosing only 84 design points. The normal recommended minimum number for constructing Gaussian process emulators is 10 per input variable, which in this case would be 130. See, for example Loepky et al, 2009, Choosing the Sample Size of a Computer Experiment: A Practical Guide, Technometrics.

P6,L30 The authors state that the choice of a linear mean function incorporates “prior beliefs” – could they explain what prior beliefs motivated this choice.

P7,L10 The authors state that the emulator error was estimated using cross validation and this is presented in the SI. However very little detail is given there except a reference to a paper describing the Matlab package used to construct the emulators (Lataniotis, 2017), which says that the package uses cross validation for parameter estimation, not emulator validation. The authors also say in the paragraph above that they used cross validation for parameter estimation. A clear statement is required as to whether or not the same cross validation was used for both parameter estimation and emulator validation. The accuracy of the emulators is of such key importance to everything that follows that summary statistics of either a separate cross validation, or a validation with a held out data set, must be presented in the main text.

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P8,L2 Could the authors comment on the validity of describing the 5km grid square containing Marylebone Rd as 'urban traffic' and the one containing N. Kensington as 'urban background'. Surely at this resolution both grid squares must be considered as urban background – this is demonstrated by the almost identical sensitivity of NO₂ and O₃ concentrations to NO_x emissions from road transport shown in figure 8.

P8,L5 The authors state that the "sensitivity indices were estimated". There are a number of published methods for doing this so could they say which method they used and why.

P14,L9 Given that O₃ concentration is known to be highly non-linear and non-monotonic in response to changes in NO_x and VOC emissions, the contention that these emulators could be used to test emission reduction scenarios is questionable as the small number of training runs used to construct the emulators means they would be unlikely to be able to accurately predict the emissions levels at which the chemical regime changes between being NO_x sensitive and VOC sensitive.

P14,L19 Could the very low sensitivity of annual mean ozone to emissions be a result of the strong diurnal variation and photochemical nature of the production of this pollutant? Could the authors comment on whether annual average 8-hour maximum might have been a more informative metric to emulate.

P14,L20 As the authors findings that variation in emissions does not cause substantial variation in the outputs contrasts with their statement in the introduction that it has been previously found that uncertainties in input emissions are major contributors to the uncertainty in the ACTM outputs, could they comment on why this might be – do they think it is a feature of the EMEP model or a result of the analysis methods?

P14,L25 Given the authors assertion in the previous paragraph that the uncertainty in model output is likely to be driven mainly by variables that they have not included in their analysis, would they concede that their uncertainty estimates are likely to underestimate by a large degree the real uncertainty in the model output, i.e. that caused

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buy uncertainty in all of the input variables plus the model discrepancy.

Interactive comment on Atmos. Chem. Phys. Discuss., <https://doi.org/10.5194/acp-2018-690>, 2018.

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