Geoscientific Model Development Discussions

Geosci. Model Dev. Discuss., referee comment RC1
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Comment on gmd-2021-39

Anonymous Referee #1

Referee comment on "Calibrating a global atmospheric chemistry transport model using Gaussian process emulation and ground-level concentrations of ozone and carbon monoxide" by Edmund Ryan and Oliver Wild, Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2021-39-RC1, 2021

This manuscript describes a method to explore sensitivity to model parameters in a global chemistry transport model using a Gaussian process emulation technique. This allows to run a large number of sensitivity experiments at a very much reduced cost compared to running those using a full chemistry transport model configuration.

Using synthetic observations, as well as (independent) reanalysis data the authors show that the method works, and provide insight in the level of spatial representation error and coverage that is needed for good parameter estimation, at least for the parameters that have been investigated in this study, namely surface O3 and CO.

This study is very well written and can be accepted for publication after the authors have addressed the following comments:

- The authors use reanalysis data from Flemming et al. (2017). It would help the reader if the authors make a clearer reference to this dataset by referring to it as the "CAMS interim Reanalysis", considering that ECMWF has published various atmospheric composition reanalyses.
  Also, even though atmospheric ozone in this reanalysis is constrained by satellite observations, the constraints on surface ozone concentrations are typically less, and are more governed by the model assumptions. To the least, it would be worthwhile to provide insight in the quality of surface ozone and carbon monoxide, e.g. as documented in Huijnen et al. (2020), and/or Flemming et al. (2017), and to what extent these aspects may alter your analysis. Also along these lines, the reference to

"measurement data" (pp 15, line 7) may be confusing in this context.

- Page 10, line 7. The authors write a little cryptically: "We included p as one of the parameters to estimate for the reanalysis data and found values in the range 0.16â□□0.19." Not being a specialist in mathematics, could you give some interpretation of this analysis? Why is it in this range, and not much smaller (or much larger)?
- Page 11, line 8: "In contrast, methods based on neural networks can require thousands of training runs.": This statement reads a bit unfounded. Could you please either add a reference (e.g. a study which actually uses a neural network approach to model atmospheric chemistry), or further clarification? If I understand correctly, one of the key aspects compared to published use of machine learning in atmospheric chemistry is that the full CTM is replaced by the Gaussian Process Emulator, rather than 'just' the chemistry solver code as I am aware of (Keller et al., 2019)
- The results from the sensitivity analysis (Sec. 3.1) indicate that surface ozone deposition is the largest driver to explain biases in modeled surface ozone concentration. While I completely understand from mathematical perspective, and experience with old-fashioned tuning in a chemistry transport model, that by changing (modifying) the dry deposition velocity for ozone has indeed a direct impact on surface concentrations, I find this result also a little worrying, in light of what would be a reasonable range of the ozone deposition flux. To get a handle on this, would it be easy and useful to quantify the change in annual total surface ozone deposition as suggested by this optimization method?
  In fact, the authors also rightly discuss the issues with this sensitivity analysis when including the simultaneous optimization of CO, pp22, line 6-9. When reading this manuscript, I had found it helpful if this aspect was already alluded to in Sec. 3.1 . Indeed, I agree that the use of this synthetic modeling can be very useful, but different optimization factors obtained using (in this case) different combinations of control variables also stress the danger of a false impression of a physically well-constrained parameter.
- Page 18, line 19: "along with a reduction in associated uncertainty": Could you be more explicit on this? I don't directly see such decrease in uncertainty.
- Figure 10, panels c/f/i : In almost any of the test configurations the parameter estimate for the Boundary Layer Mixing is approaching the maximum range that is given. Can you provide further interpretation in this aspect? Is the given uncertainty range for boundary layer mixing sufficient? Now it is written on page 21, l. 11-13 that this process "may not be represented well in the model". Or could this be an artifact of other (missing) processes not considered in this sensitivity analysis, or that this process is just treated differently between datasets.
- pp 21, l 13: "Our results suggest that dry deposition and isoprene emissions are represented relatively well in the FRSGC/UCI CTM " : Good to add phrase "with respect to the independent reanalysis data"?

Technical comment

pp 23, l9: "…while it *is* effective …"

References

Keller, C. A. and Evans, M. J.: Application of random forest regression to the calculation of gas-phase chemistry within the GEOS-Chem chemistry model v10, Geosci. Model Dev., 12, 1209–1225, https://doi.org/10.5194/gmd-12-1209-2019, 2019.

Huijnen, V., Miyazaki, K., Flemming, J., Inness, A., Sekiya, T., and Schultz, M. G.: An intercomparison of tropospheric ozone reanalysis products from CAMS, CAMS interim, TCR-1, and TCR-2, Geosci. Model Dev., 13, 1513–1544, https://doi.org/10.5194/gmd-13-1513-2020, 2020.