

Geosci. Model Dev. Discuss., referee comment RC2
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Comment on gmd-2021-26

Anonymous Referee #2

Referee comment on "Efficient ensemble generation for uncertain correlated parameters in atmospheric chemical models: a case study for biogenic emissions from EURAD-IM version 5" by Annika Vogel and Hendrik Elbern, Geosci. Model Dev. Discuss.,
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Overview:

The paper presents a method to construct ensembles with a small number (10) of members that still represent the uncertainty in ensemble applications of CTMs. The method consists of the following three steps: a) sensitivity estimation, b) eigenmode decomposition of the sensitivity information and c) generation of the ensemble based on the Karhunen-Loève expansion. The method is illustrated with the construction of an isoprene emission ensemble derived for one day.

General remarks:

The paper contains a derivation of the method in a generalised way and a discussion of its application to create an ensemble of biogenic isoprene emissions. But, it is a considerable weakness of the paper that not enough evidence is given that the ensembles generated by the method would indeed capture the main component of the uncertainty. Without this evidence, the paper has little relevance. Giving such evidence is not trivial. I can only suggest two aspects but there might be other options: 1) use the derived ensemble of isoprene emissions in an actual CTM ensemble application. 2) provide more evidence that the ensembles created using either the combined or independent sensitivities approach lead to similar results.

Of the three steps a), b) and c), a) seems to be the most interesting because it addresses the interesting questions how many model runs are required to capture the sensitivity of model result to variation of model configuration choices. By assuming linearity, the authors derive that only a reference model run and a model run with the a modification of one aspect at a time (i.e. alternative land use map, alternative deposition scheme etc.) is required and that cross-combinations of model configurations (i.e. alternative land use map AND alternative deposition scheme) are not required. Hence, the number of the required runs does not have to be all possible permutations of configuration options but only the number of tested configurations itself. Intuitively speaking, that seems obvious because the sensitivities are assumed to be linear. This means that strong non-linearities as typical for NWP dynamics or atmospheric chemistry may not be suited for the method. A better discussion of the limitations of the choice of linearity is required.

Section 2, which describes the method (a, b, c) uses a sophisticated mathematical nomenclature, which may be more confusing than enlightening for the typical GMD reader. The chapter is difficult to understand, and it should be made clearer what the main novel ideas are, and what are just mathematical definitions. For example, formulas 3a and b and 4a and b are in my opinions simple repetitions of the well known formulas for covariance and mean. I acknowledge that it is a matter of taste how "mathematical" a paper should be formulated but the mathematical formulae need to convey a specific message relevant to the objective of the paper.

The applied terms of "model argument", "model parameter", "model input" and "model implementation" are confusing. For example, I think that "model configuration" is a better term for what is meant by "model argument".

Section 3 requires more clarity on what its objective and scientific content is. For example, it should be made much clearer that one of its main purposes is to compare the combined and the independent sensitivities approach. Further, concrete evidence of the successfulness of the method (see above) should be much more the focus of that section. Finally, it would be beneficial to provide a more science-based discussion of the soundness of the derived isoprene emissions ensemble.

The discussion and conclusion section is very long. I would strongly recommend to introduce a separate and more concise conclusion section.

Figure captions need to provide more detail to make sure the figures can be understood without a lot of additional information. Acronyms in the figures should be spelled out.

Specific remarks:

I3 replace "by" with "with"

I5 make clearer what is novel about this approach (w.r.t application and method)

I12 High spatial correlation of simulated biogenic emissions is not a surprise

L 14 please compare 10 to the "uncondensed" number or ensemble member.

L 15 please provide more evidence that the 10-member ensemble indeed captures the uncertainty.

L 20-40: Most of the discussions here is on NWP ensemble construction. The aim for NWP is to get realistic error growth with increasing lead time. That is not the primary objective for the CTM applications. Perhaps you could reference here to Reduced Rank Kalman Filter approaches for CTM.

L 44 it is not just the larger state vector which distinguishes NWP from CTM ensembles but the error growth characteristics.

L 65 Please clarify what differentiates KL from singular vector decomposition methods.

L 78 Please clarify in more detail the terms "model parameters" and "model arguments" and "model inputs"

L 85 The choice of the "differently configured model simulations" is in my opinion the most interesting aspect of the paper. Please expand if this choice is guided by the algorithm or by the (human) users.

L 81 "model inputs and configurations" that are very vague terms. Please provide more detail

L 93 is it better to say the leading "un-coupled" ?

L 98 please explain here how C is related to ensemble generation

L 99 clarify "model parameters" (all model grid points, a set of 20 land use classes ?)

L 108 - is model parameter a state vector element?

L 112 It is not quite clear, why any model parameters can be considered stochastic

L 114 "i" was defined as model argument. parameters are Q (?)

L 125 is this triviality of importance later?

L 126 the log distribution may need a bit more motivation. It may be justified for positive-definite variables such as concentration but not for all possible parameters.

L 146 I do not understand the sub-sample argument here. Is not the same as choosing fewer arguments and implementations? If this is part is not referred to further down, I would simply omit it for the sake of clarity.

L 159 The assumption of linearity is an important one. It contradicts the notion that sensitivities are non-linear. This mathematical choice need to be discussed for its realism for any specific application and choice of model arguments.

L 180 I am not sure, if I understand all the need for the mathematical derivations here. Is not obvious that the assumption of linearity makes it not necessary to investigate the non-linear combined sensitivities. It seems not a result but an direct choice of assuming linearity?

L 187 The assumption of tangent-linearity might also be a strong limitation for many atmospheric applications

L 220 Please clarify what make KL superior to more standard methods to generate ensembles using singular vectors.

L 240 Was the exp transformation prone to producing unrealistically high sensitivity factors?

L 255 A bit more detail on the generalisation of the emission factors to model uncertainty parameter would be interesting.

L 255 "KL ensemble approach" I think the method is used to generate a ensemble. It is not yet an ensemble approach, which would mean the model simulation using the ensemble (emissions) itself. Please clarify what you mean.

L 265 Not clear what you mean "evaluation" ?

L 282 Please explain here that the reference is the default EURAD configuration and (2) the other configuration option.

L 285 Please discuss the plausibility of the shown sensitivity factors.

L 288 It is not clear what you mean by panel 1, 2

L 297 The additional MEGAN uncertainty might be useful for an application but for the paper it may complicate the comparison of the combined and independent sensitivities

L 324 Figure 7 should be referenced after Fig 6

L 339 The sentence is not clear. Does it mean the resulting ensemble members differ a lot between independent and combined method. That is not an evidence that the reduction in sensitivity runs works, quite the opposite.

L 361 It should be made clearer that the assumption of linearity is the main reason for reduction of the sampling space, which is no surprise.

L 366 Please clarify what you mean by "performance of the ensemble"

L 370 Please clarify, if this has been demonstrated by the presented practical results, or if this is only an assumption.

L 379 Please explain the context of the assumed number of considered arguments and realisations