Review: Quantifying the sub-grid variability of trace gases and aerosols based on WRF-Chem simulations

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General Comments:

Scientific Significance: The significance of this paper is that it addresses several critical and important modeling issues that concerns both meteorological and air quality modeling in general and for global climate modeling in particular. (1) It serves to illustrate the scale dependency of model predictions, and show clearly that this dependency also depends on the specific pollutant. (2) The paper also supports the contention that when evaluating model predictions for different pollutant species, that the responsiveness of model against observation is certainly improved when the grid size for the simulation decrease. (3) In the context of grid sizes in global or climate model simulations, this paper demonstrates that the magnitude of sub global grid scale modeling variability can be very significant, and the characteristic of this variability varies for different pollutant species, and for different transport distances from major source areas. In these regards, this is a very interesting, useful and informative paper.

Scientific Quality: In an overall perspective, the scientific quality of the work is high. However, the scope of the current study is not represented accurately by the current title. The effort reported here is self limiting to a set of formulations for use to illustrate and to begin the characterization of the fine scale structure that is inherent for grid sizes in current operational global climate models, and in this context, specifically, the WRF-Chem system, and thus limited. The general context of quantifying SGVs generically or even in light of its focus on WRF-Chem and a focus on global climate modeling is still considerably broader than its treatment here. In general, there are many aspects to quantifying SGVs, such as full distributional aspects and it bandwidth limitations based on the finest grid structure, its temporal characterization on daily, seasonal, geographical terms, as well as for its operational requirements which may differ for different targeted applications based on the range of scale of the application, e.g., climate, regional to local air quality. Thus, in this context, I strongly recommend the title of the paper be revised to more accurately reflect the study venue and scope; a suggested revised title could be "An investigation of sub-grid variability of trace gases and aerosols for global climate modeling." or something somewhat similar.

Presentation Quality: Generally good. However, some figures contain characters, too small to be legible.

The set of questions requested to be addressed in the review and my response to them are listed below:

- 1. Does the paper address relevant scientific questions within the scope of ACP? Yes
- 2. Does the paper present novel concepts, ideas, tools, or data? While not novel, there is very little t4reatment of this subject matter, thus the paper is very welcome and the outcomes are important; a qualified Yes.
- 3. Are substantial conclusions reached? Yes, for global climate modeling
- **4.** Are the scientific methods and assumptions valid and clearly outlined?
- **5.** Are the results sufficient to support the interpretations and conclusions? **Yes**
- **6.** Is the description of experiments and calculations sufficiently complete and precise to allow their reproduction by fellow scientists (traceability of results)? **Yes**
- 7. Do the authors give proper credit to related work and clearly indicate their own new/original contribution? Yes
- 8. Does the title clearly reflect the contents of the paper? No, see above discussion
- **9.** Does the abstract provide a concise and complete summary? **Yes**
- **10.** Is the overall presentation well structured and clear? **Yes**
- **11.** Is the language fluent and precise?

Yes

Yes

- **12.** Are mathematical formulae, symbols, abbreviations, and units correctly defined and used? **Perhaps (some ambiguity exists, see specific comment below)**
- **13.** Should any parts of the paper (text, formulae, figures, tables) be clarified, reduced, combined, or eliminated? **Yes, see specific comments below**
- **14.** Are the number and quality of references appropriate?

Yes

15. Is the amount and quality of supplementary material appropriate?

N/A

Overall rating of this paper: 2, but can be considered to be a 1 with suggested changes to title (discussed above) and clarification of formulation (specific comments below).

Specific comments:

- (1) Figure 3: Given the strong diurnal variation in PBL height, it would have been more illustrative to show their daytime and nighttime period average values.
- (2) The results shown in Figure 6 for aircraft transect of ozone and NOx and Figure 7 for surface time series of BC and OC provide ample reason for increasing the grid resolution of various simulations. While the point has been made, it would certainly have been interesting to show results for other pollutant species in Figure 7.
- (3) Clarification required: The definition of X bar needs to be explicitly stated; does it represent the average for each hour or the average for the entire study period. If over an hour, the SGV and SD do represent mostly the spatial subgrid, however, if it represents the period mean, the SGV and the SD will represent both the spatial and temporal variations as well.
- (4) What is SNN?

- (5) SGV descriptors are limited to included percentiles, defined SGV and SDs. The PDFs displayed for 1 (host) 75 km grid cell for the entire study period. It would be of interest to see or have indicated some aspect of the within-study temporal variability
- (6) Figure 8: Abscissa should be WRF-Chem. Unclear why the number of comparative AOD's for the 75, 15 and 3 simulations figure details were almost illegible were about the same. Shouldn't it be 25 and 625 times as many? The text did not refer nor comment on the results shown in left hand side of figure. The values for median, 25th/75th percentiles and 10th/90th percentiles on right hand side of figure were difficult to discern.
- (7) Figure 9: Please comment, if possible, the degree to which the histograms vary between the different 75 km cells, and if so, are the variations dependent on the type of pollutant, meteorological variable or terrain. Also, it would be interesting to see and have noted if and how the characteristics of the histogram changes with time of day and from day to day.
- (8) Figure 10: (a). Again, what is the X bar representing, hourly or period averages. (b) Confirm that each of the grids shown are 75 km cells.
- (9) Figure 11 and 12: The reasoning for the peak values for RH, and particulate species near the top of PBLH as largely due to the undulations of PBLH values seems reasonable and revealing given that the magnitude of SD (fig 10) were substantial.