Review 1: Quantifying the sub-grid variability of trace gases and aerosols based on WRF-Chem simulations

Authors: Y Qian, W.I. Gustafson Jr, and J.D. Fast Journal: Atmospheric Chemistry and Physics Date of Review: May 12, 2010

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 WRFChem 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."

(A) Title has been changed as: An investigation of the sub-grid variability of trace gases and aerosols for global climate modeling

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

(A) We agree that many of the figure captions are too small as presented in the ACPD draft with two figures per page. Our intent is that the multi-panel figures not be sized for a single column in

the final version. We believe the small type will not be a problem when the figures are properly sized.

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 treatment 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? Yes

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

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.

(A) The average PBL has been separated into daytime and nighttime plots (see new Figure 3) and the discussion in the text and figure caption are modified accordingly (see Section 3.1).

(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.

(A) We agree that it will be interesting to show more results for other pollutant species in Figures 6&7. Indeed we have many more of these kinds of plots on hand than are currently shown in the paper. However, based on the comments of another reviewer, Section 3 is too long, i.e. too much

space is spent comparing the model results to the observation. So, we have chosen to only add one more plot, the separate daytime and nighttime PBL plots (see specific comments 1).

(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.

(A) The x-bar is a sum over the grid points within the 75-km cell that contributed toward the standard deviation. We first calculate the SGV/SD every hour, which is the frequency of model output. Therefore the x-bar varies in time, representing the average for each hour at a particular 75-km² region. Then we average the SGV/SD over the entire time period. The text and equations in Section 4.1 of the manuscript have been modified accordingly to clarify how time averaging is handled.

(4) What is SNN?

(A) This was defined on p. 10797, line 12. However, we see how it can be confusing. We have clarified this in the text. SO4, NO3, and NH4 (sulfate+nitrate+ammonium=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.

(A) We considered including a discussion of temporal variability in the paper but chose not to do so in the original version due to the paper length. We have instead chosen to focus solely on the month average due to the scope of the paper being the variability for climate modeling purposes. We plan to address the temporal change of subgrid variability in subsequent papers.

(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.

(A) The label has been changed to WRF-Chem.

The scatter plots on the left column show the comparison between each hour that there is a valid AOD observation with the corresponding closest WRF grid point from the particular grid. So, each has the same number of points. We clarified the figure caption.

(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.

(A) Fig. 10 shows SGV spatial variability over the model domain, which can be significant. Fig. 14 shows similar results for four locations, T1 through T4, along with how the grid spacing affects the SGV for 3-km vs. 15-km spacing. While we do not show it, the temporal variability could sometimes be significant, but we have chosen to average this away for the climate aspect of our focus, as discussed above.

(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.

(A) See response for (3) for x-bar. The SGV shown is for the 3-km simulation within each 75-km grid cell from the coarser domain. The caption for Fig. 10 has been clarified.

(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.

(A) We agree.

Interactive comment on "Quantifying the sub-grid variability of trace gases and aerosols based on WRF-Chem simulations" by Y. Qian et al.

Anonymous Referee #2 Received and published: 24 June 2010

This paper contains a detailed analysis of the sub grid scale variability that could be expected in a global climate model based on results from a regional model. The scientific work is thorough and relevant to current issues in atmospheric modeling. I therefore recommend it for publication subject to the following comments below.

General Comments:

Both the abstract and the discussion would benefit from expanding the discussion of the significance and applications of the work. For example this work could be related to the common experience that performance metrics are worse with higher resolution simulations. The work on cloud variability and land use variability (Avissar and Pielke) is mentioned in passing, but seem like they could benefit from more in-depth treatment in the discussion section. One application of SGV is the chemical processing that takes place in urban plumes but cannot be represented in global models, see for example the work of M. Mayer, J. Calbo and RG. Prinn.

(A) These are very good suggestions and we have substantially added text at the beginning of the Discussion as well as in the 3rd paragraph of the Introduction to address the issues raised.

These are important comments so here we attached the contents that we added in the manuscript.

(1) Added at the beginning of the Section 6: Discussion.

"With the expected improvement of high performance computational resources, the use of high spatial resolution is perceived as a solution to partially address problems with climate simulations, including for the aerosols and their radiative forcing. How much one gains by going to very high spatial resolution modeling, however, will remain an important question. Leung and Qian (2003) suggest that increasing spatial resolution does not appear to lead to uniform improvements in precipitation and snowpack simulations over complex terrain. They found an overprediction of precipitation along windward slopes of the Cascades as model goes to higher resolution. Meanwhile their results show that errors in the snow simulation are not simply explained by elevation bias; there is a tendency for the model to grossly underpredict snow. In numerical weather forecasts for the same region, Colle et al. (1999) obtained similar findings with the resolution increasing. By analogy, these findings imply that better results cannot be guaranteed in air quality and aerosol modeling as just increasing the model spatial resolution. This is why effort needs to go into understanding the SGV.

There is also the issue of higher resolution models leading to more stringent comparisons for certain statistical comparisons. Just because the statistics look worse for higher resolution does not always mean that the model behaves worse. This is essentially the opposite of the problem raised in the preceding paragraph. For example, contingency table based metrics, such as equitable threat scores (Gandin and Murphy, 1992), that rely on "hits" and "misses" of forecasted values can have more misses for fine-scale features when simulated at high resolution. With coarser simulations, the results are smoothed out over larger areas leading to higher chances of a hit, whereas a finer grid might be closer to reality but have a feature located incorrectly. Discerning improved model behavior is therefore very difficult when

considering both the issue of true error introduced by changing the grid from error based on the analysis methodology.

Another point, that was noted in the Introduction, the SGV of trace gases and aerosols results from both the traditional subgrid processes affecting meteorology (e.g. clouds) and specific chemistry processes (e.g. emissions). Many of these processes are correlated due to mutual interactions. For example, the land use variability could potentially affect the SGV of aerosols and their precursors by changing the biogenic emissions. The vegetation can emit climate-sensitive biogenic VOCs that are oxidized in the atmosphere to form organic aerosols, or SOA. Therefore, any SGV of vegetation is related to the SGV of emissions."

(2) Added at the 3^{rd} paragraph of the Introduction.

"There are significant nonlinearities in the chemistry that arise from changing grid cell mean concentrations of gases and aerosols as a given amount of material is spread throughout a given grid cell. This issue has been known for years, but has not been adequately addressed, although there have been different attempts (e.g., Calbo et al., 1998; Mayer et al., 2000)."

There is a bit of ambiguity about the scale of features being explored. For example, Page 10780 Line 9 uses "small-scale", but this should be defined more clearly. Maybe a table of scales of different features would help. Page 10779, Line 17: "SGV is present . . . even when very small grid spacings are employed" it seems this is either redundant, or can be meaningful in terms of a discussion of feature scale.

Would it be possible to include some experimental results of SGV or of PDF to compliment the simulation results?

(A) We have added a table listing a selection of processes contributing to subgrid variability and their respective scales (see table 1). The paragraph on p. 10780 has been modified to give context to "small-scale" and to refer to the table.

Contributor to Variability	Typical Scale of Influence
Plume from point emissions	Point-like to 100 km
Plume from city	100 m to 100 km
(area and mobile) emissions	
Plume width	Function of dist. from source,10 m to 100 km
Topography & surface type variability	Function of location, e.g. smaller scale over complex topography, land-sea contrasts
Cloud-induced variability	1 km to 100 km, e.g. shallow cumulus to stratus and organized synoptic systems

We agree that observations are important to compare with the model. That is why we have spent extensive space comparing the models to available observations (Section 3). But, as explained in the response to Reviewer 1, our focus has been the spatial subgrid variability. The spatial variability cannot be quantified from the surface observations because of their lack of site density.

The best opportunity would be to use satellite data, which is beyond the scope of this project. We have a proposal under review at this time specifically addressing this need.

In general, I found sections 3 and 4 to be longer than they needed to be with the message swamped in details. If anything, Section 5 and 6 could maybe be adjusted to bring out the implications of the results more clearly.

(A) We have refined some of Section 3 to reduce its length and additions from other comments for Sections 5 & 6 help highlight relevant issues.

Specific Comments:

Doesn't WRF use "eta" not "sigma" levels?

(A) WRF uses a sigma-like terrain following coordinate system that is represented by the character η . This coordinate system is different from the Eta coordinate system used in the Eta model. We changed the word "sigma" to " η " in the caption of Fig. 11.

Page 10779, Line 23: full stop after "western US"

(A) You are correct. The editor removed the periods from "U.S." in our submission and created the problem. We will look for this error closely in the final manuscript in case it happens again.

Page 10779, Line 26: "effectively extrapolate" was not clear to me what this means exactly.

(A) This sentence has been reworded.

Page 10796, Line 11: I thought that SD was the root of the square of the differences – the exponent is missing.

(A) Fixed.

Page 10800, Line 10,11: Specie*s*? MOSAIC not MOSIAC

(A) "Species" is both singular and plural, e.g. see http://dictionary.reference.com/browse/species. Fixed MOSAIC—thanks.

Page 10804, Line 22-23: "The SGV for C3 is larger than for C15" – wouldn't you expect this by definition? Given the model set-up, would it not be more accurate to talk about the SGV at 75km based on the C3 simulation. It seems that this is a further example of the need to discuss the scale of simulated features more thoroughly.

(A) For a fully converged model grid, i.e. the results no longer change with increased resolution, the increased SGV for C3 would not occur. For example, if one were doing flow over an airplane wing, which has a fixed forcing scale, at some point a resolution would be reached that no further detail would be added at higher resolution. However, you are right that for most

atmospheric models, which never truly converge for any practical resolution, it is an almost foregone conclusion that SGV for C3 would be larger than for C15.

Note that the SGV for C3 and C15 is an index based on the variability within a 75-km² region. So, it is a measure of the subgrid variability within a 75-km² region as resolved by the 3 or 15-km grid.

In response to the issue of scales raised above, we have added the new table showing example subgrid forcings, and have also added some related discussion in the text.

Page 10806, Line 26-27: This is to be expected given that emissions take place during the day, and so presumably background / air mixed on a larger scale dominates at night?

(A) This is an interesting comment. Additional discussion has been added at the end of Section 5.1. See below what we added:

"This last point is interesting in that it represents a balance between processes operating on differing spatial and time scales that impact the SGV. For a given region, there is a diurnal cycle and spatial distribution associated with the emissions. The emissions are typically lower during nighttime. But simultaneously, PBL mixing is also minimum at night. This leads to the spatial structure imposed by the small-scale emission sources being maintained, and thus the impact on SGV of the emissions. Alternatively during the day, the emissions are typically higher, which implies a greater contribution to the SGV from the emissions. However, mixing within the PBL is also higher during the day, which would work to smooth out the spatial gradients, and thus reduce the SGV. Because the simulated SGV is actually stronger during the day, this implies that the increased mixing within the PBL is insufficient to counteract the higher emission rates. Whether or not this is a universal finding, or is specific to the Mexico City area, is unknown."

Page 10807, Line 28 - 1: Again, it seems that this is fairly obvious (surface impact of terrain), but what is the implication of this?

(A) Although the qualitative conclusion can be expected here, in this section we quantify the impact of terrain on SGV and compare this with the impact induced by emission. The first paragraph of this section has been expanded to give some context. See below what we added: "The PBL evolution and regional flows, which are strongly affected by topography, have a significant impact on pollutant dispersion. Importantly, this impact is nonlinear and not easily generalized. For example, just because there is a lot of variability in the terrain height within a given grid cell, one cannot know *a priori* what the bias will be on the flow and PBL structure. The direction of mountain ridges or valleys within the cell, in combination with how these connect to features in neighboring grid cells, and the current meteorological conditions, will alter the terrain induced SGV for a given cell. "

Page 10812, Line 1-4: see note for pg 10804 above. You are approximating the SGV at 75km using simulations at 3km and 15km. The text is not entirely clear about this. It seems that the finer the simulations used to estimate the SGV, the larger the results would be?

(A) Yes, as explained in the response for 10804, until convergence is reached, it appears that the magnitude of SGV generally increases with the spatial resolution of the model. We have modified the text to clarify that, except for Section 4.6, the SGV is usually calculated based on the 3-km simulation within each 75-km grid cell from the coarser domain.