### Authors' response to the review comments

Title: OMI NO<sub>2</sub> column densities over North American urban cities: The effect of satellite footprint resolution

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First of all, the authors express their appreciation to the two reviewers and the editor. We believe that their comments are very productive and substantially contributed to improving the manuscript. We offer point-by-point responses to the issues and comments addressed by reviewers. Reviews' comments are shown in italics.

### Reviewer #1

"The manuscript addresses an innovative way of enhancing the spatial resolution of OMI NO2 columns for studies of the urban plumes in the US by adopting the spatial distributions of the NO2 columns from the CMAQ model. Another important point the manuscript emphasizes is careful ways of processing the satellite retrievals and model results for quantitative comparisons that were often neglected. The IDL-based routine developed in this study (Figure 3) will be useful for many users of OMI retrievals. I suggest the authors to share this routine with potential users through the GMD journal."

We thank the reviewer. We will include the IDL routines of "conservative spatial regridding" and "downscaling" of OMI and CMAQ NO<sub>2</sub> VCDs in the supplementary materials with brief descriptions. Users will be able to download and test sample codes, and further modify the codes for their own interest.

### "\* Page 8457, Figure 4: An interpolation routine should be applied to make plots in Figure 4 from Figure 3. I suggest the authors to explain this part. It would be helpful if the names of cities in the text are given on the map."

Thanks for the comment. We have included city names on the NO<sub>2</sub> VCD spatial plots.

In order to convert irregular-shaped satellite data into model grid, we use a conservative spatial regridding technique based on polygon clipping algorithms instead of a traditional interpolation method. We have included descriptions of the method below. More detailed descriptions can be found in Kim et al. (2013).

Regridding of model output or satellite data with different map projection settings is very important for inter-comparisons of modeled results and/or satellite outputs. Spatial regridding is a commonly performed procedure in satellite data processing. It converts a data set between different map projections and resolutions. Among numerous spatial regridding methods, interpolation and pixel aggregation are two of the most common methods. Interpolation is preferred when the target domain resolution is finer than that of the raw data pixels, on the other hand, pixel aggregation is the preferred way to average all the pixels inside each domain cell when the grid cell size is bigger than the raw data pixel size. Despite their popularity, both methodologies for interpolation and aggregation have numerical limitation especially in dealing with fine resolution data and/or where conservation of

measured quantities is required. More mathematically complete methods for spatial regridding is to handle the geospatial data (e.g. satellite data) as "polygon with area" instead of "(dimensionless) pixels". It requires the calculation of fractional areas between the overlapping polygons that describe raw data pixels and modeling grid cells.

The IDL-based Geospatial Data Processor can provide exact fractions using the polygon clipping algorithm, and this information can be used for lossless (zero-loss) spatial regridding in the conservative remapping method. This method reconstructs raw data pixels (e.g. satellite data) into target domain grid cells, by calculating fractional weighting of each overlapping portions between data pixels and domain grid cells. If the raw pixel data is in density units (e.g. concentration) we can calculate the overlapping fractions for each data pixel and grid cell. The grid cell concentration can be calculated as a weighted average of data pixels and fractions. (Fig. R1)

$$f_{i,j} = \frac{Area(P_i \cap C_j)}{Area(C_j)}$$
$$C_j = \frac{\sum P_i \cdot f_{i,j}}{\sum f_{i,j}}$$

where i and j are indices of data pixel, P, and grid cells, C.  $f_{i,j}$  is the overlapping fractions, and  $\sum f_{i,j}=1$  if no missing pixels are involved in grid cell  $C_j$ .

If the satellite pixel data is in mass units, equations for the conservative remapping are slightly different. We need to calculate fractions of overlapped area to raw data pixel size, instead of grid cell size.

$$g_{i,j} = \frac{Area(P_i \cap C_j)}{Area(P_j)}$$
$$C_j = \sum P_i \cdot g_{i,j}$$

where  $g_{i,j}$  is the fraction of overlapped area to the data pixel size.



Figure R1. Example of "Conservative spatial regridding" method using variable-pixel linear reconstruction algorithm

"\* Page 8459, line 17-19: I think the emission problems are large and that certainly affect the spatial distribution of the plumes. In addition to wind errors, the impact of emission inventory errors from various sectors can be large (see Figures 8 and 10 in the manuscript). Potential problems stemming from this error source need to be written clearly. And which emission inventory was utilized for the model simulations? This may determine the limit of the methodology developed in this study."

Thanks for the comment. We agree that emission information plays a crucial role in the technique described in this study. We have included the descriptions for emission used in the model run. Detailed information on the emission data is also described in (Pan et al., 2014).

We have clarified the limitations of current downscaling technique. As described in line 178-192, this method can be affected if an emission source has any error in its geospatial information. On the other hand, this method is less sensitive to the absolute strength of emissions from known sources. It is an unique advantage of the conservative downscaling technique of this study. Further investigations on the technique using different emission data, different meteorology and/or chemistry model are being conducted, but the results are not included in the current draft yet.

# "\* Page 8460: I think it is best to show the comparison results for other days (May 7, May 16 etc.) and discuss the causes for agreement or disagreement. Was P3 data averaged for comparison with OMI data (at a model resolution)? Was averaging kernel applied to P3 data?"

Thanks for the comment. Figure 6 already includes measurements from all three days (May 4<sup>th</sup>, 7<sup>th</sup> & 16<sup>th</sup> 2010), and we have clarified it. Spatial plots of the original and adjusted OMI NO<sub>2</sub> VCDs for all days are shown in the Figure R2. Clear enhancements are shown in May 4<sup>th</sup> & 7<sup>th</sup> when the P3 measurements show strong spatial gradient, and the impact is weaker on May 16<sup>th</sup> 2010 when its spatial gradient is smoother (Sunday, less traffic due to the weekend effect). Current P3 circles represent averages of OMI pixel's coverage since they were initially prepared for a direct comparison between OMI and P3 NO<sub>2</sub> VCDs (Judd et al., in preparation)

Since observations (e.g. OMI and P3) are column-integrated 2 dimensional data and model has 3 dimensional structures, we applied the averaging kernel information to 3 dimensional model structure and converted the model  $NO_2$  concentration into column data (2 dimensional) format (e.g.  $NO_2$  VCD) for the comparison with observations. OMI and P3 are compared directly.



Figure R2. Comparisons of spatial distributions of OMI and P3 NO2 VCDs for May 4<sup>th</sup>, 7<sup>th</sup>, & 15<sup>th</sup>, 2010.

# "\* Page 8462: For Figure 9, the period of analysis needs to be given in the main text. The results in this manuscript are based on a short-term analysis. Please mention this clearly in the many plots and analyses in the manuscript. Explain the differences in Figure 9d. Which points show large discrepancies between the OMI data and the model results in Figure 9d?"

Thanks for the comment. We have included that Figure 9 is for a one month period of September 2013. In addition, we like to note that we have tested all months in 2013 & 2014. Their results are mostly consistent.

Since this study mainly focuses on the uncertainty of satellite to model comparison due to spatial resolution differences between satellite footprint pixels and model grid cells, we did not emphasize on the implication of the comparison. However, we notice that the comparison in this draft shows general agreement with previous research. For urban locations (e.g. higher NO<sub>2</sub> VCD values), the trend of continuous NO<sub>x</sub> emissions reduction, especially from the mobile sources, might be the main reason of the overestimated CMAQ NO<sub>2</sub> VCDs. On the other hand, the underestimation of CMAQ NO<sub>2</sub> VCDs in the rural areas (e.g. lower NO<sub>2</sub> VCD points) might be attributed to the lack of natural NO<sub>x</sub> emission sources in the current modeling system, especially the soil NO<sub>x</sub> emissions. It also should be noted the rural NO<sub>2</sub>

VCD level is usually near the lower boundary of detection limit from space-borne instrument, so satellite-based measurements have relatively high uncertainty in the rural area.

## *"\** Page 8463, line 5-6: it is not clear that the recent shale-gas development is a significant source of NOx. One even assumes zero emission from this source. I could not find a reference (Chang et al., 2015) in the reference section."

Thanks for the comment. Although the emission from recent shale-gas development is a very important topic, we agree that there is no clear consensus on detailed information on those emissions yet, and they are beyond the scope of this study. We have clarified it in the main context.

### "\* Figure 10: Discuss causes for the differences between the OMI data and the model results."

Thanks for the comment. We have included additional discussions on the causes of discrepancies between OMI and modeled NO2 VCDs. As already mentioned for the comment on Figure 9, the reduction trend of urban NOx emission (e.g., mobile sources) might be the main reason of the overestimated CMAQ NO2 VCDs. On the other hand, missing natural NOx emission sources in rural area could be the reason for the underestimation of CMAQ NO<sub>2</sub> VCDs.

### *"\* Acknowledgements: The P3 data from the CalNex campaign and related scientists should be acknowledged."*

Thanks for the comment. We have included acknowledge for the P3 campaign and scientists.

Thanks again for very productive comments.

### Reviewer #2

The authors express their appreciation to the reviewer. We provide replies for the reviewer's two main comments: (1) Why this draft is suited to the GMD's general goal, and (2) why findings and approaches in this draft are valuable for the future scientific model development. We also try to clarify the use of Averaging Kernel (AK) in the draft. Reviews' comments are shown in italics.

(1) The journal choice

### "I consider this study out-of-scope for the aforementioned journal, as the authors have merely used the CMAQ model in their study; the study does not include any aspects of model development."

We believe that the evaluation of a model is a crucial part of model development. Without proper evaluation with observational evidences, the model's capability to represent the natural phenomena will be seriously limited. The main goal of this study is to discuss how a geoscientific model should be evaluated when its evaluation has likely been systematically biased due to data resolution.

In this draft, we have demonstrated that a direct comparison of the modeled and satellite NO<sub>2</sub> vertical column density (VCD) over urban cities might have serious systematic bias due to differences in the data geospatial resolutions between the model and observation (e.g. satellite). Subsequently we have described an approach to reduce this systematic bias. We have submitted this draft to the *Geoscientific Model Development* because our study addresses the scientific fairness in model evaluation between different geospatial data sets. This is a fundamental underpinning of model development.

Furthermore, the comparison of modeled and satellite  $NO_2$  VCDs is usually used to improve model's emission input (e.g.,  $NO_x$  emission) which is one of the most important elements for better atmospheric chemistry modeling system.

(2) Scientific importance and implication

### "The study lacks scientific novelty. Regarding the second point, the fact that measurements of trop. NO2 over urban areas are not able to capture the high pollution maxima over the emission hot spot due to the spatial smoothing caused by the coarse satellite ground pixel is trivial and has been reported on previously."

The reviewer commented that this draft is trivial since the underestimation of satellite  $NO_2$  VCD observations over urban cities due to its coarse spatial resolution has already been reported. However, this comment seriously misinterprets our work. The draft did not only report these biases, but also tried to quantify the magnitude of the biases, and tried to suggest approaches to overcome those systematic biases.

In addition, we do not agree with the notion that quantification of such biases as was suggested by this draft is trivial or negligible. The draft has demonstrated that the theoretical systematic biases from OMI could be as large as 100% over urban cities just by the geometric effect of coarse satellite footprint pixels. Considering the economic cost and impact on the public health, the estimation suggested from this study has a serious implication in the interpretation of current anthropogenic emission inventory, and should be further considered in the policy decision-making of emission regulation.

For more detailed technical point of view, this study is a first approach to use a (mass) conservative spatial regridding method with satellite data in a footprint pixel level (e.g. level2), using the polygon clipping algorithms. Although the smoothing effect due to satellite resolution is already reported, there have been few approaches to adjust the impact of satellite resolution effect; Hilboll et al. (2013) might be the one of the few to name. In accordance with the authors' knowledge, no approach has been tried with pixel level mass conservation in the top-down approach.

The key idea in this approach is to handle geospatial data as "polygon with area" instead of "pixels", as described in Kim et al., (2013) or in the response to the review #1. The mass conservative spatial regridding capability will be essential in the development of fine-scaling modeling approaches. We believe that this technique can provide a useful tool to handle multi-scale model or geospatial data together; It can be useful for the comparison between model and satellites, or inter-comparison between various satellite platforms.

### "The fact that the agreement between modelled and measured pixels improves when AK information is applied to the model fields is also trivial; in fact, any quantitative comparison between model and measurements has to use AK information, as neglecting to do so leads to a comparison of apples and oranges."

Moreover, we would like to clarify the use of the Averaging Kernel (AK) information. We <u>do not claim</u> that the use of the AK information in the comparison of modeled and space-borne NO<sub>2</sub> VCD is one of our achievements in this study. We just used the AK information because its use is a necessary step to prepare the satellite data for a fair comparison as the reviewer commented. We described through a step-by-step data comparisons (e.g. raw data case, using AK case, using downscaling (DS) case, and using both AK and DS case), to demonstrate that the impact of the DS method is comparable to the impact of AK use in the model-satellite comparison. If one thinks the use of the AK is mandatary for satellite-model comparison, we suggest that the impact of satellite footprint pixel resolution also should be considered to understand the fine scale phenomena such as urban NO<sub>2</sub> plumes.

Thanks again for the reviewer's comment.

### References

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