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Interactive comment on "A sub-grid model for improving the spatial resolution of air quality modelling at a European scale" *by* Mark R. Theobald et al.

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Updated Authors' response to the comments by Anonymous Referees #1 and #2

We would first like to thank both referees for their useful and constructive comments. We have combined the responses to both Anonymous Referees and the responses have been grouped by topic to improve readability. Page and line numbers refer to the manuscript version with Tracked Changes (provided as a supplement to these comments).

Approach used

Ref#1: Referring to this technique as 'modeling the sub grid scale variability' is mis-

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Discussion paper

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leading because there is nothing in the formulation of the CTM that has been changed here to actually model the unresolved variability. In my view, what they develop is a post-processing, downscaling technique to map regional scale simulations on finer resolution emission data using some parametrization to account for dispersion of these emissions.

Ref#1: The parametrization of emission dispersion does not include any sub grid process such as fast chemistry or deposition. What is more, the time scale of their application is much coarser than the CTM's (annual vs. several minutes though the time step of the EMEP model is not explicitly mentioned). Those choices make it clear, in my opinion, that this effort is not meant to solve the subgrid variability. To do so, the effort would rather focus on high resolution meteorology and emissions on line with the regional CTM to capture the unresolved features of atmospheric chemistry and dispersion.

Authors' response: We appreciate the referee's opinion on this matter. We think that it is a question of definitions. The referee's interpretation of the term "sub-grid model" appears to be that of a parameterisation within a coarse resolution model (e.g. a CTM) that explicitly takes into account sub-grid variability during the simulation. We use the term "sub-grid model" to mean a parameterisation that can refine the outputs of a coarse resolution model, by providing an estimate of the spatial distribution of the model output (e.g. atmospheric concentrations) within each grid cell of the coarser model. In this respect we a using the term "sub-grid model" in the same sense as that used by various publications cited in the manuscript (Ching et al., 2006; Denby et al., 2011; Dragosits et al., 2002 and Isakov et al., 2007). The manuscript has been revised to clarify what we mean by sub-grid modelling (see e.g. p 4 lines 13-14).

Ref#2: I have difficulties understanding why NO2 photochemistry is not needed here. By using the NOx fine-scale emission pattern and distribution kernel for redistributing NO2 concentrations this approach assumes a constant NO2/NOx concentration ratio in the whole EMEP 50km grid cell, which is hard for me to believe. Typically this

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ratio should show a dip close to NOx sources due to the high NO ratio in primary emissions. Also this fraction of primary NO2 in NOx emissions varies strongly between different sources and this should play a role at the local scale. I thought that at least ADMS includes a NOx photochemistry formulation, why is this not used? Ideally such a chemistry scheme should be used, or at least the potential errors discussed. Along similar lines, also the formation of NH4 can influence local NH3 concentrations – it would be interesting to know what the potential errors are when these processes are ignored.

Authors' response: The assumption of a constant NO2/NOx concentration ratio is made to provide a simple parameterisation that is universally applicable. It would be difficult to include a variable ratio in a simple model since it would depend on the local pollution climate (e.g. ozone concentrations), photochemical reactions of NO and NO2 emitted from the different source types and complex variations in diurnal emission patterns and meteorological drivers. Both AERMOD and ADMS include optional simple photochemistry schemes but they depend on background ozone concentrations, which are not homogeneous across the domains, and so these model options cannot be used for developing a simple generic model, which was the aim of the study.

Of course this simplification will introduce uncertainty into the model. This uncertainty can be estimated by analysing the variability of the NO2/NOx ratio in the measured data. For the Scottish domain, the coefficient of variation of the ratio is 20% whereas for the Dutch domain it is only 7.5%. Estimating the NO2 concentrations from the measured NOx concentrations, assuming a constant ratio, gives mean errors (NMGE) of 18% and 6.3%, for the Scottish and Dutch domains, respectively. Extending this analysis to the annual mean concentrations for the sites in the European air pollution database "airbase" that simultaneously measure NO and NO2 (1478 sites), gives a coefficient of variation of 17.5% and a mean error of 14.6%. Based on the European dataset, we estimate that the mean error introduced by assuming a constant NO2/NOx ratio is about 16%. A discussion of these uncertainties has been included in the Dis-

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cussion section (p 12 lines 23-28).

Similarly the formation of NH4+ from NH3 depends on the concentrations of other pollutants, as well as the complex variations in diurnal emission patterns and meteorological drivers, the inclusion of which is beyond the scope of a simple sub-grid model. However, a discussion of the uncertainty due to this omission has been included in the Discussion section (p 12 line 28 to p 13 line 1).

Ref#1: How would results look like if no dispersion was taken into account and the same process was done only by using the 1km (or 7km or both) emission proxy?

Authors' response: We have now included these analyses using the 1 x 1 km2 emission data for both NO2 and NH3 (p 10 lines 6-15 and Figure 6). As now mentioned in the discussion, these results show that short-range dispersion estimates are necessary for improving on the EMEP model predictions.

Meteorological data

Ref#2: I find it hard to understand why meteorological data from just one station was used here, instead of grid-specific meteorology consistent with the fields driving the CTM. Even the two "domain-specific" meteorological data sets come only from one station each. I think this needs to be better justified and compared to the effects a grid specific met data set would have.

Ref#2: Since the authors mention this as a possibility I would suggest that they add a sensitivity analysis using grid-specific meteorology consistent with the CTM

Ref#1: Wouldn't it make more sense to use the same meteorology as in the EMEP model at least for this sensitivity test?

Authors' response: The model was developed using a single meteorological dataset to provide a simple parameterisation that could be of benefit to the wider air quality modelling community. The model was tested with meteorology specific to each modelling domain to show that the model results were not that sensitive to the meteorological

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data set used. However, we agree that it makes more sense to use the same meteorology as the EMEP model and we have done this for the revised manuscript. The original approach using the modified meteorological data from just one station is now included as a sensitivity test and is now referred to as the simulation using "synthetic meteorological data". As can be seen in Figure 5, the use of the EMEP model meteorology does not make a large difference to the concentration predictions and model performance is similar, strengthening the conclusion that the approach is fairly insensitive to the meteorological dataset used. The manuscript has been revised to reflect this change in methodology (see e.g. p5 lines 5-12; p 7 lines 7-8 and lines 17-19).

Ref#2: Why is it justified to assume rotationally symmetric dispersion kernels, should not the local predominant wind direction have a significant influence? How big is the error introduced by this rotationally symmetric formulation?

Authors' response: In order to keep the model parameterisation simple and universally applicable, we decided to remove the influence of local wind direction distributions (which are not valid for the whole domain) by assuming rotationally symmetric dispersion kernels. It can anyway be noted that in the real world local wind-directions will differ from that of a larger scale model. For example, cities are frequently located in locations subject to topographic (e.g. valley) winds, or sea-breezes. Although this rotation symmetry obviously does introduce some error, the results shown in Figs. 4 and 5 demonstrate that even with this assumption the sub-grid model provides a valuable improvement over that of the larger scale CTM. The use of EMEP model meteorology, however, now relegates this approach to that of a sensitivity test.

Emissions

Ref#1: I am wondering what do emission sources as large as 1km2 could possibly represent. In my understanding, dispersion models are conceived to represent emission from point sources such as industrial stacks. Is this the right model to represent large area sources such as crops or residential emissions? Is this type of modeling adequate

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to represent dispersion around busy roads? Don't dispersion patterns depend on the emission sector?

Authors' response: The use of 1 km2 emission sources is a simplification due to the fact that we do not have emission inventories for the study domains at a higher spatial resolution. So in reality we may have a large point source within a specific 1 x 1 km2 grid cell but since we do not know exactly where, we distribute this emission over the whole grid cell. Of course this is a simplification which is going to introduce uncertainty in the model but it is the best we can do with the available emission data. The model, therefore, would not be expected to be suitable for estimating concentrations close to busy roads but the model performs well for the Dutch traffic sites. This has been made clearer in the revised manuscript (p 13 lines 5-11).

Averaging period

Ref#1: It would be interesting to look at the effect of the meteorological dataset at a finer time-scale. Especially since the authors claim in their conclusions that this method is easily applicable at finer time scales.

Authors' response: As stated in the manuscript, the annual mean limit values for NO2 are generally more stringent than the hourly ones and impacts of NH3 are only assessed using annual mean concentrations. We agree that it would be interesting to develop a model with a higher temporal resolution, but such a study would raise other issues (e.g. as discussed above, or with the availability and accuracy of time-resolved emissions). Thus, we did not consider this to be 'easily applicable' at finer time-scales, but rather, as we state in the discussion, this is a potential future improvement and is out of the scope of the presented work.

Model evaluation

Ref#1: I don't think it is appropriate to say that "the sub grid model performed better than the EMEP model". It would be more fair to say that the downscaled version of the

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EMEP model compares better with observations.

Authors' response: This is a fair point and the manuscript has been modified accordingly.

Ref#2: Does this mean the downscaling decreased agreement to NO2 non-traffic stations, which are the ones we would actually expect it to improve? As mentioned above, I would not expect the 1x1km model to be representative of traffic stations.

Authors' response: You would expect the sub-grid model to perform best for the non-traffic stations but for the Dutch domain it had the lowest bias and error for the traffic sites. This suggests that the model may be suitable for simulating concentrations at traffic stations, providing they are located several metres from the roadside (as is the case for most of the Dutch sites), and the good agreement is likely the result of the fact that the majority of roadside sites are not situated along isolated motorways, but rather embedded in urban areas with dense road networks. This is now highlighted in the Discussion (p 13 lines 8-10).

Manuscript structure

Ref#2: I would find it helpful if the downscaling equations were written out as equations and not only described verbally

Ref#2: Why moving window? Is the final subgrid distribution pattern at a given 1km grid cell not simply made up from the sum of all emissions times kernel within the range of the kernel? Perhaps a better formulation could be to say that the kernels are not cut off at the EMEP grid boundaries (I hope). Again, formulating this with equations would help here.

Authors' response: This is a good suggestion and the downscaling equation is now included in the Model Development section. The dispersion kernels are not cut-off at the EMEP grid boundaries. This is now clarified in the description of the downscaling equation (p 7 lines 26-27).

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Miscellaneous comments

Ref#1: The inevitable question arises of whether a direct EMEP run at 7km resolution with its corresponding meteorology would bring about the same improvement as the downscaling developed in the present study. And in this case the data would be directly at hourly resolution.

Authors' response: Although it is currently possible to run the EMEP model at a 7 km resolution for specific projects, they are far too CPU intensive for routine use, and especially where CTMs need to be run 10s-100s of time for emission control assessments. However even at a spatial resolution of 7 km, the EMEP model would not be able to resolve the large horizontal concentration gradients found close to sources and a subgrid treatment may still be necessary. This is now clarified in the Introduction (p 3 lines 15-16).

Ref#2: One issue that is not addressed here nor anywhere else in the manuscript is that (to my understanding) the lowest vertical layer of the EMEP model extends from the surface to about 90 meters. In this context, it would be important to explain what is meant by 'the mean atmospheric concentration in each grid square': Is this the estimated surface concentration calculated by applying some standard vertical distribution? But if so, is it then justified to assume that the modelled mean concentration on the 50km grid is 'correct' and just needs to be re-distributed spatially within the grid cell?

Authors' response: The EMEP model estimates the near surface concentrations by extrapolating the concentration at the mid height of the first vertical layer (45 m) assuming an approximately constant vertical deposition flux. Of course, there are uncertainties in this procedure, especially for NH3 where deposition velocities can be relatively high, but where bi-directional exchange complicates even the sign of atmosphere-biosphere exchange in real situations. However, we have to work with the EMEP values as provided by the model, and our working assumption is that the errors in the vertical dis-

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tribution are less important than the errors we seek to minimise – namely those of sub-grid horizontal variability. This is now clarified in the Introduction (p 2 lines 20-22).

Ref#1: If the mean value is correct it would be surprising that the urban background concentration is underestimated. It would make sense to say that near-sources concentration levels are under predicted but if the background value is off as well, I don't see how we could get the mean value right.

Authors' response: Although this comment refers to the conclusions stated by Denby et al. (2011), we will attempt to respond to the referee′s comment. Both rural and urban areas can be present within a 50 km grid square of the EMEP model and so it is possible that the model predicts the correct mean value for the entire grid square but underestimates concentrations within the urban area (at both traffic and background locations). This would be the case, for example, if the rural area occupies the majority of the grid square.

Ref#1: If I think that the comparison with Denby et al., 2011 study is off mainly because they worked on hourly data and not annual.

Authors' response: We disagree with this comment because the study of Denby et al. (2011) is based on annual mean concentrations.

Ref#1: If I think that the correlation in Schaap et al., 2015 is on time and not in space as in the present study.

Authors' response: We are referring to Figure 7 of Schaap et al. (2015), which is included in the section on spatial analysis (although it appears to be erroneously referred to as "temporal analysis" in the figure caption).

Ref#2: In case of PM10 to my knowledge the limit on daily means (35 exceedances of 50ug/m3) is the more stringent one.

Authors' response: Yes the referee is correct, for PM10 the limit for daily means is the more stringent one. The reference to PM10 has been removed from the revised

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manuscript (p 12 line 17)

Ref#2: I wonder whether the quotes are really necessary here.

Authors' response: Maybe not for the "moving window" but we think that the quotes necessarily highlight the new term "sub-grid distributions" in order to distinguish it from the term "sub-grid concentrations".

Ref#2: SO4-2 should be SO-24?

Authors' response: Yes, that is correct and the change has been made.

Ref#2: Figure 4: I would suggest to split up the two regions into separate figures, since the model performance is so different.

Authors' response: We agree and the figures for the individual domains have now been included in the supplementary material.

Additional changes to the manuscript

In addition to the changes mentioned above, the following additional modification has been made to the manuscript:

- The model name and version has been included in the manuscript title, as per journal guidelines and the model name and acronym used throughout the manuscript

Please also note the supplement to this comment:
http://www.geosci-model-dev-discuss.net/gmd-2016-160/gmd-2016-160-AC3-supplement.pdf

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