Interactive comment on “WRF-chem model predictions of the regional impacts of $\text{N}_2\text{O}_5$ heterogeneous processes on nighttime chemistry over north-western Europe” by D. Lowe et al.

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What is the justification behind the choice of 15x15km in the horizontal directions? The results from flight measurements seem to indicate that narrower pollutant plumes were observed, could the model be able reproduce those plumes if the resolution was finer?

The resolution of 15 km was chosen for the grid as a compromise between the competing demands of having a domain which is large enough that it includes the major sources of pollution within the region which might influence the study area (so we need to cover the whole of the UK, the North Sea, the Netherlands and Belgium, and large
parts of Germany and France); and which is fine enough resolution that the aircraft flight path is not covered by just one or two grid cells, but is coarse enough that running the (reasonably) highly detailed chemistry scheme is not too expensive.

At the start of setting up the study we did plan for the 15 km resolution domain to be just the outer domain for a nested grid, with a 5 km resolution domain over the general region of the flights, in order to capture small-scale features such as the pollutant plumes. The position of this second domain relative to the first is shown in Figure 1.

During the process of developing and testing the model chemical schemes, inputs, and configuration, we did some (small-scale) tests of the impact that this increase in resolution would have on our model skill. Table 1 and Figure 2 show the results of one such test, where we compared the statistical fit of the model predictions for the 15 km and 5 km resolution domains with the 1-minute averaged measurement data along the flight path for flight B535 for key gas-phase species. For this test we ran the inner domain off-line (using the WRF-Chem off-line nesting utility, ndown), starting from midnight on the 16th July 2010 (giving 45 hours spin-up time for the inner domain before the flight started), and with full $N_2O_5$ heterogeneous chemistry. Our model setup was not fully finalized at this point (nor had we ironed out all of our coding bugs) so the model predictions for the 15 km domain are a little different to those that we present in the paper — however they are sufficiently close to the final model results, and fully internally consistent, to allow us to use them for this demonstration.

The differences in mean value calculated from the two model domains is less than 1% for $O_3$, and less than 3% for NO$_2$, NO$_3$, and N$_2$O$_5$. These differences are significantly smaller than the differences between the model and the measurements (see Table 1). Similarly, the correlations of the model predictions for each domain with the measurements are very similar (see Figure 2; circles and diamonds indicate results from the 15 km and 5 km resolution domains, respectively), with only the correlations for NO$_2$ (blue symbols) and N$_2$O$_5$ (green symbols) increasing on the higher resolution domain (and even then, not by much). There is greater heterogeneity in the 5 km domain.
results, as demonstrated by the (small) increases in the standard deviations of NO₂, NO₃ (red symbols) and N₂O₅, but the increase in model detail did not result in a significant increase in the model predictive skill. This is similar to the results from previous studies, which have shown that the spatial match between measurements and model predictions of plumes is much more difficult to get right at high grid resolutions (≈ 1 km) (c.f. Fast et al, 2006).

Because of the model skill was not significantly improved by the higher resolution, and because using a higher model resolution would have increased our computational costs (at least) by a factor ≈ 3–5, we decided, for the final study, to use only the outer, 15 km resolution, domain.

Reference:

Measurements | 15 km grid | 5 km grid
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O₃ (ppbv) | 33.4 | 36.9 | 37.2
NO₂ (ppbv) | 1.64 | 1.48 | 1.52
NO₃ (pptv) | 23.4 | 32.0 | 32.7
N₂O₅ (pptv) | 154 | 233 | 238

Table 1. Mean values from 1-minute averaged measurements, and model data, along the flight track of flight B535.
Fig. 1. Position of the inner, 5~km grid-resolution, domain within the outer, 15~km grid-resolution, domain.
Fig. 2. Standard deviations of, and correlations between, model and measurements along flight track. Circles and diamonds indicate results from 15 and 5 km grids, respectively. See text for more details.