Authors' reply to comments of Referee 2

We thank Referee 2 for the very helpful feedback on the manuscript. In the following, we address the comments, listing the Referee's comment (bold), our response (normal font) and changes in the manuscript, if applicable (indented). All references given in this response can be found in the bibliography of the discussion paper or below each response. In addition to the changes replying to the Referees' comments, we made few further minor changes to the manuscript, listed below.

RC2-I

You used the RADM2 mechanism. This mechanism doesn't include several important biogenic VOCs, therefore it usually underestimates ozone compared to such gas chemistry mechanisms as RACM. I suggest this point to be discussed in the paper.

RADM2 is a mechanism that is frequently used. We include a discussion of this as well as possible reasons for biases in ozone related to the chemical mechanism in the manuscript as follows.

> Page 4, line 29 – page 5, line 1: "The setup includes the RADM2 chemical mechanism with the Kinetic PreProcessor (KPP) and the MADE/SORGAM aerosol scheme. RADM2 has been used frequently in air quality applications over Europe (Mar et al., 2016, Im et al., 2015, Tuccella et al., 2014); the effect of this choice of chemical mechanism on modeled concentrations is further discussed in Section 4.2.1."
>
> Page 14, line 5-7: "This is consistent with what has been reported for a coarse European domain using RADM2 chemistry (Mar et al., 2016) and in line with previous studies showing a deficiency of many online-coupled models, including WRF-Chem with the RADM2 chemical mechanism, in simulating peak ozone concentrations (e.g. Im et al., 2015a). Mar et al. (2016) suggested that the low bias in modeled ozone could be partially explained by the inorganic rate coefficients used in the RADM2 mechanism."

RC2 – II

You used 35 vertical levels, how thick is the first layer? You did simulations as high as 1km resolution, which certainly helps to capture spatial variability of the urban canopy and anthropogenic emissions in more detail. However, the vertical resolution remained the same. I think relatively coarse vertical resolution could explain some of the model deficiencies, especially the nighttime bias in the model.

The first layer is at ca. 30m above the surface. We will add this information to the model description. Mar et al. (2016) have tested increasing the vertical model resolution and found that surface layer concentrations do not change much. For further discussion of the vertical model resolution as well as changes in the manuscript on the topic of vertical resolution please see our reply to the comments of Referee 1 ("general concern", "comment on page 10, lines 1-17", "summary").

> P. 4, line 28-29: "The model top is at 50 hPa, using 35 vertical levels. The first model layer is at approximately 30m above the surface, with 12 levels in the first 3km. "

RC2 - III

Chapter 2.1- doesn't the ERA-INTERIM have 61 vertical levels?

The full dataset has 60 vertical levels (http://www.ecmwf.int/en/what-vertical-resolution-data). Here, we used the data interpolated to pressure levels. We made this clearer in the text as follows.

> Page 5, line 2-4: "We use the European Centre for Medium-Range Forecast (ECMWF) Interim reanalysis (ERA-Interim, Dee et al., 2011) with a horizontal resolution of 0.75°x0.75°, temporal resolution of 6h, interpolated to 37 pressure levels (with 29 levels below 50 hPa), as meteorological initial and lateral boundary conditions."

RC2 - IV

2.2- WRF also uses more updated MODIS LU dataset. Here the USGS LU data is mentioned only.

Thank you for pointing this out, we added it in the text.

Page 5, lines 9-10: “An analysis of the USGS land use data commonly used in WRF showed that the land cover of the region around Berlin is not represented well. In addition, the MODIS land use dataset as implemented in the WRF-Model from v3.6 only includes one category classifying urban areas. “

RC2 – V

2.4- The stack height could be small, but the plume injection height due to buoyancy and momentum is higher. I think this could explain some of the NOx overestimations by the model at nighttime, when all the NOx from the point sources are emitted into shallow boundary layers.

Thank you for your comment, we agree with you. We included this in the discussion of the original manuscript, e.g. page 19, lines 3-6: “As for the vertical distribution of emissions, Mar et al. (2016) state it has little impact on the model results. While this might hold for simulations of rural background air quality with domain resolutions of the order of 45km, the present results suggest that it is of higher relevance to distribute point source emissions into several vertical model levels when decreasing the model resolution and the resolution of the emission input data. “ In addition, we elaborate further on this responding to the comments of Referee 1 (e.g. response to “RC1 - Summary”).

RC2 – VI

In WRF-Chem the vertical mixing of the chemical species are done somewhat differently than the meteorological fields. Did you consider testing sensitivity of the vertical mixing of the chemical species to various parameters/assumptions? The treatment of vertical mixing of the chemical species can explain some of the high NOx bias at night.

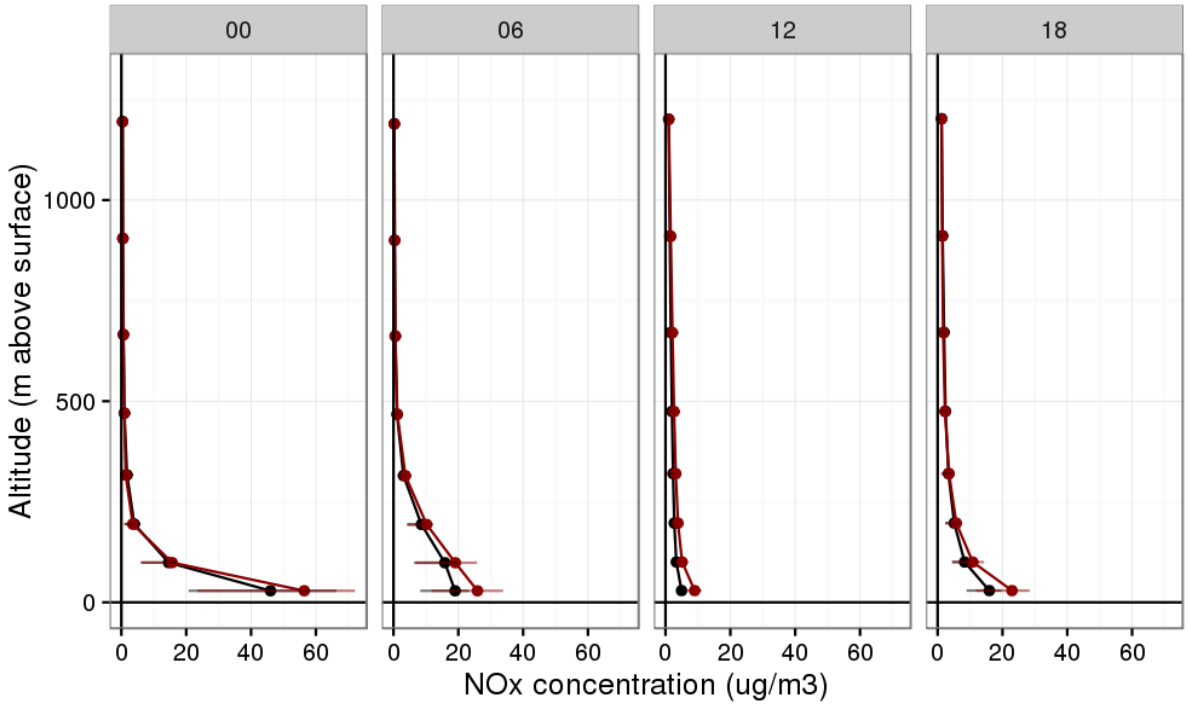
We did not test the sensitivity of the vertical mixing of the chemical species to different parameters/assumptions for this study, as its main focus was to evaluate the model and test the sensitivity of the results to model resolution, resolution of the emission inventory as well as input parameters to the urban scheme and land use input data. However, we discuss the vertical mixing as a potential cause of the NOx bias at nighttime, e.g. page 13, lines 12-13: “The main reason for the nighttime overestimation is likely the model’s underestimation of nighttime mixing […]”. In addition, please also see our discussion in response to the comments of Referee 1 concerning the vertical resolution of the model (e.g. response to “General Concern”, response to “RC1- Summary”).

RC2 – VII

In addition, I suggest showing vertical profiles or x-sections of the chemical species (e.g. NOx) to illustrate how deep the species were mixed in the model, especially during nighttime.

Thank you for your suggestion. We have included exemplary vertical profiles in the supplement (see figures below). The figure shows mean NOx profiles in the lower troposphere simulated with a 1kmx1km model resolution at 00:00, 06:00, 12:00 and 18:00 UTC, for the base run (black) and S3 (downscaled emissions, red), for Amrumer Straße. Error bars give the 25th and 75th percentiles. We also included the following description in the manuscript:

Page 13, from line 12: “The main reason for the nighttime overestimation is likely the model’s underestimation of nighttime mixing as discussed above. This is supported by the vertical distribution of NOx at several locations in the urban area, which shows a strong gradient between the first and second model layer (e.g. figure S10 in the supplementary material as an example).“



RC2 - VIII

Can you show model-obs. comparisons similar to Figure 11 for NOy (if measurements are available) as well? The paper doesn't show any evaluations for CO, biogenic VOCs such as isoprene etc.

Unfortunately, measurements of NOy are not available. We do also not have observations of CO for urban background stations in Berlin for 2014. We agree with you that a comparison of modeled with observed CO might help to get additional insight into the cause of the NOx-bias and will consider this for further analyses. These are, however, beyond the scope of the present study. As for the comparison with VOCs, Churkina et al. (in preparation) compared modeled with observed isoprene and find that isoprene in the urban background is simulated reasonably well, but underestimated in urban parks and forests. The manuscript of Churkina et al. will include a detailed discussion of this comparison.

Further changes

Page 2, line 14-15:

The limit value was not exceeded at 3 stations instead of 1 station.

> "In Berlin, measured NO2 annual means exceeded the European limit value of the annual mean at all but three measurement sites close to traffic in 2014 […]"

Page 7, line 2-4:

The sentence "All emissions from the energy industry..." is somewhat unclear and was changed to

> "In the TNO-MACC III inventory, all emissions from the energy industry within Berlin are point sources, and of the emissions from other industry sectors ca. 55% of the total emissions within Berlin for CO, 9-17% for particulate matter and up to 1% for other gases are included as point sources."

Page 11, line 7-8:

There is a typo in this paragraph, it will be changed to

"[…] while the bias of maximum temperatures modeled with 3km and 1km resolutions is mainly positive, the bias of the maximum temperatures modeled with a 15km resolution is negative."

References

The manuscript of Jänicke et al. (2016) has been accepted for publication.

The reference of Tuccella et al. (2012) had a typo and was corrected.

The references mentioned in the response to the referees were added to the bibliography.