

# ***Interactive comment on “Ozone air quality simulations with WRF-Chem (v3.5.1) over Europe: Model evaluation and chemical mechanism comparison” by K. A. Mar et al.***

**K. A. Mar et al.**

kathleen.mar@iass-potsdam.de

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The authors would like to thank Anonymous Referee #2 for their constructive comments. Below are our responses.

1) lines 50-52: The authors give here three examples of air quality models but maybe they could also refer here to the review article of Baklanov et al. (2014) for the online coupled regional meteorology chemistry models in Europe.

The original manuscript did include a citation to Baklanov et al. 2014 (line 53-54). However, we have added in the revised manuscript a more detailed reference to this manuscript: “The application of online coupled regional meteorology chemistry models

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in Europe, among them WRF-Chem, has been recently reviewed by Baklanov et al. [2014].”

2) lines 62-64: The importance of time variant chemical boundary conditions for simulated near surface ozone over Europe has been also highlighted in other recent regional modelling studies (see e.g. Akritidis et al., 2013).

Following the referee’s suggestion, the manuscript has been extended, mentioning a the importance of temporally varying chemical boundary conditions.

“The importance of temporally varying chemical boundary conditions in air quality modeling has also been stressed in other studies (including Akritidis et al., 2013; Andersson et al., 2015).”

3) line 264: Please provide some more information on the selection of the AirBase stations classified as rural background. Do you include stations with class 1–3 according to the Joly-Peuch classification methodology for surface ozone (Joly and Peuch, 2012). This approach has been also applied in a recent study by Katragkou et al. (2015) for the evaluation of MACC reanalysis near-surface ozone over Europe.

We used the classification of stations provided with the metadata in AirBase. This is now indicated in the revised manuscript in Section 3.2.2.

“Because of the relatively coarse horizontal resolution in this model study, model output is only compared against AirBase stations that are classified as "rural background." The station classification was taken from the metadata provided by the EEA for AirBase.”

4) line 283: You may add one sentence with information for the use and value of SOMO35 index.

A brief discussion of the purpose and use of the SOMO35 metric has been added to the manuscript in Section 3.3.

“SOMO35 is an indicator of cumulative annual ozone exposure used in health impact

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assessments. The accumulated health impact is assumed to be proportional to the sum of concentrations above a cutoff of 35 ppb, chosen because the relationship between O<sub>3</sub> and adverse effects is very uncertain below this threshold (WHO, 2013).”

5) Looking the Figures 4 and 9 I am wondering why at the lateral boundaries there are such differences between the two simulations with the different chemical mechanisms (RADM2 and MOZART) even though they are constrained with identical O<sub>3</sub> chemical lateral boundary conditions.

The importance of ozone import into the model domain from the lateral boundary conditions depends not only the concentration at the lateral boundary conditions (as the reviewer notes, in the case of MOZART and RADM2 simulations, these concentrations are the same), but also on the dominant wind flows at the edge of the domain. A plot of seasonally averaged wind vectors from ERA-Interim for 2007, which are the fields used to force model meteorology at the edges of our domain, has been added to the Supplementary Material (Figure S2). The dominant flow of air onto the European continent is from the west, and we see that the western (particularly northwestern) edge of the domain is where seasonally-averaged O<sub>3</sub> values are most similar between the MOZART and RADM2 simulations. At the northwestern edges of the domain, we see that seasonal average O<sub>3</sub> predicted by RADM2 is generally not more than 5% lower than that predicted by MOZART. At the southern and eastern edges of the domain, there is not a strong flow of air into the model domain, which dampens the impact of ozone boundary conditions in this area.

In addition to the addition of Figure S2 to the Supplementary Material, we have made the following addition to the text in Section 4.2.1.

“Absolute O<sub>3</sub> concentrations are most similar (i.e., less than 5% different) between the mechanisms near the northwest edges of the domain (see Figures 4 and 9), where the prevailing westerly winds (Supplementary Material, Figure S2) mean that O<sub>3</sub> imported from the boundary conditions plays a dominant role.”

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6) lines 546-551: Normally with NO<sub>x</sub> titration we mean the first order removal process of O<sub>3</sub> through direct reaction with NO which takes place during nighttime and in the vicinity of large NO emission sources. However the presented results refer to summer daytime and maybe this behaviour is related to the saturated NO<sub>x</sub> conditions (or VOC sensitive conditions) in these areas (which is a different issue). The split between NO<sub>x</sub>-saturated or NO<sub>x</sub>-sensitive regimes is driven by the chemistry of odd hydrogen radicals with HNO<sub>3</sub> being the dominant sink in the first case and peroxides the dominant sink in the second case. Maybe the authors could also plot the photochemical regimes in their simulations for the month of July using VOC/NO<sub>x</sub> or H<sub>2</sub>O<sub>2</sub>/NO<sub>y</sub> ratios (see also the study of Beekmann and Vautard, ACP, 2010).

The reviewer is correct; in this discussion the term "NO<sub>x</sub> titration behavior" has been replaced with "NO<sub>x</sub> saturated behavior." Regarding plotting chemical indicators for chemical regime, an additional plot showing the indicator CH<sub>2</sub>O/NO<sub>y</sub> has been added to the Supplementary Material (Figure S12); a brief discussion of this figure is now included in Section 4.3. A comparison of our results on NO<sub>x</sub> vs. VOC sensitivity to the findings of Beekman and Vautard (2010) has also been added to the discussion. The revised discussion is copied below.

"Notably, the U.K., Benelux, northern France and Paris, and northwest Germany show NO<sub>x</sub>-saturated behavior, in which increased NO<sub>x</sub> emissions lead to decreased O<sub>3</sub> concentrations. NO<sub>x</sub>-saturated regimes are also seen around the area of the Mediterranean between Monaco, Genoa and Corsica. An alternate approach to identify areas of NO<sub>x</sub>-sensitive vs. NO<sub>x</sub>-saturated regimes is to use indicator ratios (in the base simulation) following Sillman (1995). We have applied this approach with the indicator ratio CH<sub>2</sub>O/NO<sub>y</sub> (Figure S12) and find that areas identified as NO<sub>x</sub> sensitive using the indicator ratio are the same as those identified using the simulation with +30% NO<sub>x</sub> emissions. These results are also consistent with the areas of Europe found to be NO<sub>x</sub> saturated in the model study of Beekmann and Vautard (2010). Magnitudes of the observed change in O<sub>3</sub> in response to increased NO<sub>x</sub> emissions are quite similar for both

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mechanisms, although RADM2 shows slightly stronger NO<sub>x</sub> saturation (i.e., a stronger decrease in O<sub>3</sub> given a 30% increase in NO<sub>x</sub> emissions) in the area centered around Benelux, and stronger NO<sub>x</sub> sensitivity over Scandinavia and northwest Russia.”

7) lines 558-559: Mind also that the highest sensitivity for ozone production with regards to VOC is at the regions of high NO<sub>x</sub> emissions as someone would expect for the regions in the VOC limited regime.

We see that in areas with high NO<sub>x</sub> emissions such as Benelux, northern France and Germany, and shipping tracks in the Mediterranean, both RADM2 and MOZART predict VOC-sensitive conditions. This point have been added to the discussion in the revised manuscript. However, the increases in O<sub>3</sub> with +30% VOC emissions are still relatively small. The text has been updated as follows:

“Areas where MOZART and RADM2 are in agreement in predicting VOC sensitivity (increased O<sub>3</sub> concentrations in response to increased VOC emissions) are generally those with high NO<sub>x</sub> emissions, where one would expect the highest VOC sensitivity based on theory; these areas include Benelux, northern France, northwest Germany, and shipping tracks in the Mediterranean. However, the increase in O<sub>3</sub> concentration is modest for both mechanisms; for RADM2 it is generally limited to increases of 2-4% over the base simulation.”

8) lines 565-566: Do you think that the different O<sub>3</sub> sensitivity to VOC changes in the two schemes can account for the O<sub>3</sub> differences between RADM2 and MOZART (e.g. the lower ozone values in MOZART)? If yes, in which sense?

The results of the +30% VOC sensitivity studies for July (Figure 16) indicate that  $d[\text{O}_3]/d[\text{VOC}]$  is higher (more positive) for RADM2 than for MOZART for the chemical regime represented by the models in July 2007. This is an indication that the two mechanisms are simulating different O<sub>3</sub> chemical regimes – in the case of RADM2, there is a greater extent of VOC sensitivity, which means that addition of VOC emissions moves the chemistry in the direction of maximum O<sub>3</sub> production efficiency, which

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is not the case for MOZART over much of the domain. A more extensive study would be needed to evaluate whether the conclusion that  $d[\text{O}_3]/d[\text{VOC}]$  is higher for RADM2 than for MOZART can be applied more generally. In our simulations, this effect (i.e., more O<sub>3</sub> incremental production from VOC in RADM2 than in MOZART) appears to be dominated by other differences between the mechanisms (e.g., the inorganic rate coefficients), given that O<sub>3</sub> concentrations predicted by MOZART are always greater than those predicted by RADM2 in our simulations. A discussion of this has been added to Section 4.3:

“The results of the +30% VOC sensitivity studies for July indicate that  $d[\text{O}_3]/d[\text{VOC}]$  is higher (more positive) for RADM2 than for MOZART for the chemical regime represented by the models in July 2007. This shows that the two mechanisms are simulating different O<sub>3</sub> chemical regimes – in the case of RADM2, there is greater VOC sensitivity, meaning that addition of VOC emissions moves the chemistry in the direction of maximum O<sub>3</sub> production efficiency; this is not the case for MOZART over much of the domain. A more extensive study would be needed to evaluate whether the conclusion that  $d[\text{O}_3]/d[\text{VOC}]$  is higher for RADM2 than for MOZART can be applied more generally.”

9) lines 575-578: This is an interesting result which shows that differences in rate constants can account by 40% for the O<sub>3</sub> differences between RADM2 and MOZART runs. You may highlight this result a bit more.

This result has been highlighted further in the Abstract and in the Summary and Conclusions. In the Summary and Conclusions section, we further suggest that harmonization of inorganic rate constants could potentially lead to reduced spread in predicted O<sub>3</sub> among multi-model studies such as AQMEII. In the abstract, discussion of this difference now reads: "Additionally, we found that differences in reaction rate coefficients for inorganic gas phase chemistry in MOZART- 4 vs. RADM2 accounted for a difference of  $8 \mu\text{g m}^{-3}$ , or 40% of the summertime difference in O<sub>3</sub> predicted by the two mechanisms."

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In the Summary and Conclusions, the text has been updated as follows. The first sentence was in the original manuscript, the second sentence has been added.

“Although the most fundamental differences between MOZART- 4 and RADM2 (and other chemical mechanisms used in regional modeling) is the representation of VOC oxidation chemistry, we find that approximately 40% of the difference seen in predicted O<sub>3</sub> seen in this study can be explained by differences in inorganic reaction rate coefficients employed by MOZART- 4 and RADM2. This result suggests that harmonization of inorganic rate coefficients among chemical mechanisms used for regional air quality modeling might be valuable, and could potentially lead to a smaller spread in model-predicted O<sub>3</sub> compared to that seen in, e.g., the multi-model studies of AQMEII (Solazzo et al., 2012b; Im et al., 2015).”

10) lines 591-594: Taking into consideration all three (rate constants, deposition and photolysis schemes) it seems that altogether account about 60% for the O<sub>3</sub> differences between RADM2 and MOZART runs. Is this correct? You may highlight this conclusion.

It is true that if one looks at the average change in O<sub>3</sub> concentration in these three sensitivity simulations, then a total of 60% of the MOZART-RADM2 difference in O<sub>3</sub> concentration is explained, assuming that the effects are additive. However, the authors have consciously avoided presenting this as a conclusion in the text; since the effects of inorganic rate constants, photolysis and deposition are highly interconnected, it is reasonable to assume their combined effects may not be simply additive. We consider a quantification of the nonlinearity of this behavior to be outside the scope of this study.

11) Figure 3: I guess here the authors refer to wind direction. Please also provide information on the approach calculating the wind direction difference between obs and model.

The caption for Figure 3 has been fixed and now correctly refers to wind direction rather than wind speed. A more detailed description of how modeled wind direction was compared to observed wind direction has been added to Section 3.3, and reads

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as follows.

“When applying these statistics to wind direction, wind direction was treated as a scalar quantity, when in fact it is a vector. This simple approach was favored rather than applying a correction (as done by, e.g., Zhang et al. (2013a) in cases where the difference in modeled vs. observed wind direction were greater than 180°). This is not expected to make an important impact on our analysis, especially since northerly winds (i.e., centered around 0°, or equivalently 360°) are not prevalent in Europe (see Figure 3 and Figure S2 in the Supplementary Material).”

12) Figure 16: Maybe it would be better to show the sensitivity result in a percentage scale (from -10 to 10 %).

In Figure 16, the plot has been adjusted to show the percent difference rather than the fractional difference.

Minor comments line 209: delete double "and". line 239: It is "for" instead of "fo". line 305: Maybe "related" instead of "associated" . line 406: It is "configuration" instead of " configuruation".

All of the above minor comments have been addressed with corrections in the text.

lines 427-429: The sentence needs rephrasing. It is not clear.

The sentence now reads "Coates et al. (2016) have shown that adding representation of stagnant conditions (which were not represented in Knote et al. (2015)) to a box model increased the sensitivity of predicted O3 to the chemical mechanism, and also improved model agreement with observations."

We believe this has improved the clarity of the original sentence, which read "Coates et al. (2016) have shown that accounting for stagnant conditions in a box model increased the variability in predicted O3 with temperature in a way that better reproduced the variability seen in observational datasets and 3-D model simulations; adding representation of stagnant conditions (which were not represented in Knote et al. (2015)) to the

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box model also increased the sensitivity of predicted O<sub>3</sub> to the chemical mechanism."

Interactive comment on Geosci. Model Dev. Discuss., doi:10.5194/gmd-2016-131, 2016.

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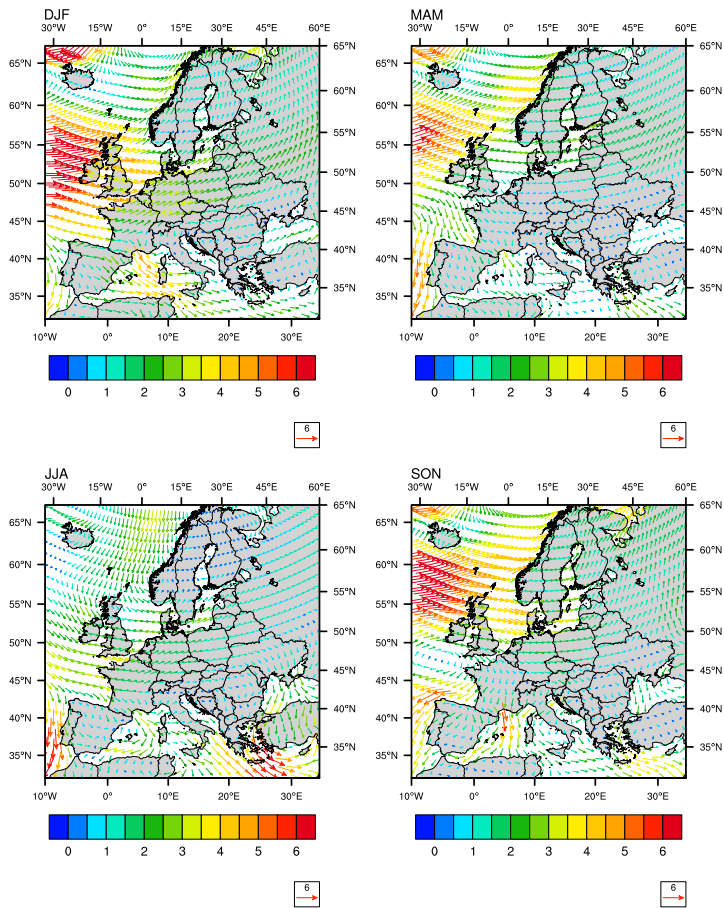
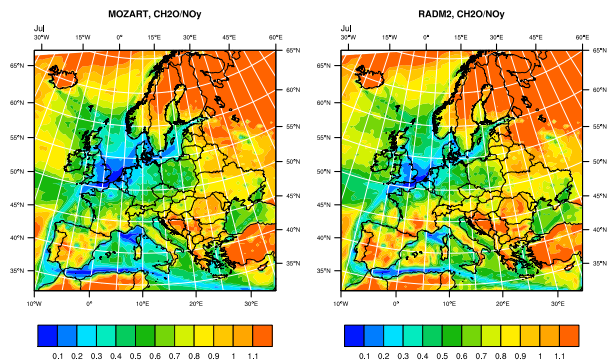


Fig. 1. Figure S2, Seasonally-Averaged Wind Vectors from ERA-Interim

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**Fig. 2.** Figure S12, CH<sub>2</sub>O/NO<sub>y</sub> indicator for July sensitivity run

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