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Interactive comment on "Development of an atmospheric chemistry model coupled to the PALM model system 6.0: Implementation and first applications" *by* Basit Khan et al.

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Discussion paper

Response to comments of the anonymous Referee #2, "RC2"

The paper describes the new PALM6.0 model system, an extension of the existing PALM model with on-line gas-phase chemistry (several schemes, with different levels of complexity) and deposition. The functioning of the system is evaluated for the different chemical schemes for test cases in Berlin. In addition the computational costs of the different levels of complexity are analysed. The paper is quite well-structured and complete. Case studies are interpreted in detail and compared to observations. Figures are relevant and to the point. All relevant aspects are described. However, at some places further clarification is needed. Also the English needs improvement. All in all I compliment the authors with their nice work and I'm looking forward to the final version.

Author's resp: First of all, we want to thank the reviewer for the effort in reviewing our paper and the valuable detailed comments, which helped us to improve the paper. Please note that page and line numbers mentioned in responses to comments correspond to the updated version of the manuscript.

Detailed comments

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Discussion paper

Comment: Abstract Since you name the chemical mechanisms at the end of the abstract you can also directly name them in the beginning of the abstract and rank them in complexity. Naming of emission mode is not so relevant here. The authors state that this is the first paper with complex gas phase chemistry at this high resolution in an on-line coupled model for an urban geometry. However, the feedback of modelled concentrations on meteorology is not elaborated here. The authors could say a few words on this.
Author's resp:: We have modified the abstract accordingly.

Comment: P3: Li et al 2016 also included rather detailed chemistry, but indeed more simple than CBM-IV
Author's resp:: A reference to Li et al. (2016) was already included in the submitted paper. However, we agree that the reference to this paper should be more visible and the sentence "The NCAR LES model with coupled MOZART2.2 chemistry (Kim et al., 2012) includes a quite detailed description of isoprene oxidation and its products. This model was also applied by Li et al. (2016) in order to investigate turbulence-driven segregation of isoprene over a forest area with a grid with of 150 m" has been added (Pg 3, Ln 13-14).

Comment: P7: CBM-IV is replaced by more detailed CB5 and CB6 mechanisms, so not that widely used any more, but you could give the valid argument that it is the lightest version of 'full' gas-phase chemistry.
Author's resp: We modified the text accordingly (Pg 7,Ln 15-16).

Comment: P8 l20 confusing sentence, compounds are not all in the particulate phase
Author's resp: We changed the sentence to " Currently the full SALSA implementation in PALM includes the following chemical compounds in the particulate phase: sulphate (SO_4^{2+}), organic carbon (OC), black carbon (BC), nitrate (NO_3^-), ammonium

(NH_4^+), sea salt, dust and water (H_2O)" (Pg 8, Ln 12-14).

Comment: P11 Numerical set-up description. The authors switching between description of case, used observations and numerical set-up makes it more difficult to follow or look things up.
Author's resp: We have re-organised this section completely. Subsection 3.1 also renamed as " Modelled episode and modelling domain". Two further subsections have been introduced in order to improve the readability of this section (Pg 11-14 Ln –).

Comment: P11 L8 It was not a weekend, therefore, emissions from the traffic were not affected by the reduced trafic Which reduced traffic? You mean that the day is a working day with the corresponding traffic activity, which is higher than in a weekend. The topic is addressed better on p 11 and p13. This sentence is confusing
Author's resp: The sentence has been modified as "July 17 2017 was a Monday, therefore, the diurnal cycle of the traffic emissions can be described by a typical weekday with relative maxima during the morning and evening rush hours." (Pg 11, Ln 6-7).

Comment: P 12 L3-4 in one sentence 50 and 60 m used, why this criterium? What is a few?
Author's resp: We have modified the sentence and mentioned the number of high buildings: 'With the exception of 10 buildings with a height between 45 m and 65 m and two buildings, which are higher than 70 m, the building heights in the simulation domain are between 5 and 45 m." (Pg 11, Ln 15-16).

Comment: P13 Observed NO, NO2 and O3 from Berlin city, are these the stations in section 3.2? Did you interpolate or take one value for the domain?

Author's resp: Yes, we used values from this network. This is explained more clearly now in the text and we added a remark, that all grid points of the domain are initialised with identical pollutant profiles (Pg 14, Ln 17-18).

Comment: P15: This part about chemistry needs some reformulation and better explanations. R3 should also contain an M on the left side.
Author's resp: Thanks for making us aware of the missing M. The reaction R3 and some text in this section has been updated (Pg 16, Ln 9).

Comment: P16 l6 The authors state that NO and NO2 do not lead to a net gain in O3. But that is not completely true, the final photostationary equilibrium depends on NO2/NO ratio and changing emissions/concentration leads to a change in O3, as correctly stated on p18l12. VOC plays an additional role. For an urban area with NOx abundance, VOC is mostly the limiting factor for O3 formation. Also in R4, the meaning of RH and RO2 are not explained in the text. The additional impact of VOC is indeed visible in Figure 10.
Author's resp: We have added a remark that ozone production is possible by emission and subsequent photolysis of primary NO_2. RH and RO2 are now explained (Pg 17, Ln 6-13).

Comment: P17, section 4.3 Spatial distribution of pollutants: why do you switch to CBM4 here, whereas SMOG was the chosen to be the default chemical scheme? 4.2 was with SMOG (as I understood from the context and the model description: SMOG was chosen. . .p13 l8)
Author's resp: We are sorry that we did not mention properly that the baseline case was performed with CBM4. We have added the sentence "Assuming that CBM4 is more accurate than the more simple mechanisms due to its more complete representation of atmospheric chemistry, the baseline simulation of this study was

performed with CBM4." Furthermore, the mechanism used is now also mentioned in the figure captions (Pg 13, Ln 27-29).

Comment: P22 l 28 Downwelling in the entrainment zone: I would call this entrainment, mixing in of air when the boundary layer rises. See also p24 last sentence.
Author's resp: This sentence has been rephrased (Pg 23, Ln 13-14).

Comment: P24 l 18 Missing emission sources: would you expect that the contributions from industry, household and BVOC would have a significant peak in the evening in summer? I doubt this.
Author's resp: We agree and have removed this sentence (Pg 25, Ln 19-20).

Comment: P25 Section 4.6 Numerical efficiency test, are case A and B related to a specific location? Is domain A included in B, for which day?
Author's resp: Yes, the smaller model domain of Case A is included in B. This is now also mentioned in the text (Pg 27, Ln 8-9).

Comment: P27 Concluding remarks. Now that the chemistry schemes are compared in terms of performance with respect to observations and computational effort, could you conclude whether SMOG or CBM-IV would be the best default option? Especially in the light of the further complexity of the model (BVOC, SALSA) and the last sentence. How does your conclusion relate to practices in other LES models?
Author's resp: We added a further paragraph to the conclusions, which addresses this issue (Pg 29, Ln 16-24).

Comment: Typo's/text corrections
a. P10 l6 sentence with mostly sunny with. . .

b. L 16 Ceilometere
c. P22 l 31-32 Although. . .., however. . . Use one of the two
d. P14 output-> put out/written to file. Output was exported to file every 10 minutes. . ..
Author's resp: Thanks for making us aware of typos and suggestions for improvement. The text is updated (a. Pg 11, Ln 5; b. Pg 12, Ln 11; c. Pg 23, Ln 17; d. Pg 15, Ln 4).

Comment: P10: Meteo from web sources: this is meteo from the airport published at a website I assume. When I read the sentence I'm in doubt of the data source and quality.
Author's resp: We have replaced the reference by a better reference, which refers to the same data. We have also mentioned that the metéo data are from Berlin Tegel airport (Pg 12, Ln 8-9).

Comment: P11, p12 Some brackets missing in references
Author's resp: Missing brackets added. Pg 12, Ln 9,10

Comment: P12 L9-11 confusing and..and.. with respectively, unclear what is meant exactly
Author's resp: There was indeed something wrong with this sentence. We replaced it by "Trees resolved by the canopy model are characterised by the three-dimensional leaf area density per unit volume (LAD). For the model configuration used here, LAD is considered for, i.e. up to a maximum height of 40 m above the ground and assumes values up to 3.1 m^2 m^{-3} with an average value of 0.44 m^2 m^{-3}." (Pg 12, Ln 1-4).

References

Kim, S.-W., Barth, M C., Trainer M., 2012:Influence of fair-weather cumulus clouds on isoprene chemistry.*Journal of Geophysical Research: Atmospheres*,**117**. doi:10.1029/2011JD017099.

Li, Y., Barth, M.C., Chen, G., Patton, E.G., Kim, Si-Wan., Wisthaler, A., Mikoviny, T., Fried, A., Clark, R., Steiner, A L., 2016:Large-eddy simulation of biogenic VOC chemistry during the DISCOVER-AQ 2011 campaign.*Journal of Geophysical Research: Atmospheres*,**121**(13,) 8083-8105. doi:10.1002/2016JD024942.