

## ***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.***

### **Anonymous Referee #2**

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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.

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#### Detailed comments

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.

P3: comment: Li et al 2016 also included rather detailed chemistry, but indeed more simple than CBM-IV

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.

P8 l20 confusing sentence, compounds are not all in the particulate phase

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.

P11 L8 It was not a weekend, therefore, emissions from the traffic were not affected by the reduced traffic. 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

P 12 L3-4 in one sentence 50 and 60 m used, why this criterium? What is a few?

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?

P15: This part about chemistry needs some reformulation and better explanations. R3 should also contain an M on the left side. P16 l6 The authors state that NO and NO2 do

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not lead to a net gain in O<sub>3</sub>. But that is not completely true, the final photostationary equilibrium depends on NO<sub>2</sub>/NO ratio and changing emissions/concentration leads to a change in O<sub>3</sub>, as correctly stated on p18112. VOC plays an additional role. For an urban area with NO<sub>x</sub> abundance, VOC is mostly the limiting factor for O<sub>3</sub> formation. Also in R4, the meaning of RH and RO<sub>2</sub> are not explained in the text. The additional impact of VOC is indeed visible in Figure 10.

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)

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.

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.

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?

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?

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

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.

L 16 Ceilometere

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P11, p12 Some brackets missing in references

P12 L9-11 confusing and..and.. with respectively, unclear what is meant exactly

P14 output-> put out/written to file. Output was exported to file every 10 minutes. . .

P22 l 31-32 Although. . ., however. . . Use one of the two

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