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Geoscientific Model Development Discussions

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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Response to comments of the anonymous Referee #1, "RC1"

Comment (1): The current manuscript describes a new city-scale LES-Chem model, PALM-4U and presents test simulation results with a variety of chemistry modules. It is indeed important to have a variety of chemistry modules from simple to complex in one model, so that each user can allocate limited computational resources to his/her own specific targets. Some might need higher resolutions or longer time integrations, while some might need very accurate chemical modules for coarser resolutions or shorter time integrations. The quality of their work meets the standard of GMDD but there are several issues remained to improve the presentation of manuscript as listed in the following specific comments.

Author's resp: First of all, we would like 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 attached updated version of the manuscript

Comment (1) The country names are missing in the affiliations of co-authors from #2 to #6.
Author's resp: Country names have been added to the affiliation text.

Comment(2) There are several abbreviations in abstract without being defined, such as PALM, PARAMETERIZED, CBM4, SMOG, and PHSTAT. PALM is their model name but it is never spelled out throughout the manuscript.
Author's resp: PALM, and chemistry mechanisms have now been defined when the first time they appear in the text. Emission mode 'PARAMETERIZED' is defined briefly in the abstract and then in greater detail in section 2.3 (Pg 1, Ln 2, Ln 8-10, Pg 10, Ln 1-2).
"...PALM model system 6.0 (formerly an abbreviation for Parallelized Large-eddy Simulation Model and now an independent name)... "
"... ranging from the photostationary state (PHSTAT) to mechanisms with a strongly simplified VOC chemistry(e.g. the SMOG mechanism from KPP) and the Carbon bond mechanism (CBM4, Gery et al. (1989b)), which includes major pollutants namely O3, NO, NO2, CO, a more comprehensive, but still simplified VOC chemistry and several products ... "

Comment(3) There are more abbreviations in the entire manuscript, such as MITRAS, ASMUS, SALSA, etc. Better to spell them out when they appeared first time, or make a table of nomenclature.
Author's resp: Abbreviations have been spelled out in the text (Pg 2, Ln 31-32; Pg 4, Ln 9).
"...and trees e.g. MITRAS (the microscale obstacle resolving transport and stream model), (Salim et al., 2018) and ASMUS (A numerical model for simulations of wind and pollutant dispersion around individual buildings), (Gross, 1997),..."
"... SALSA (A sectional aerosol module for large scale applications), (Kokkola et al., 2008) implemented in PALM ..."

Comment(4) The relationship or difference between PALM and PALM-4U is unclear in

the entire manuscript. Sometimes the author write PALM, but sometimes PALM-4U. It can be read that PALM consists of PALM-4U and the chemistry module was in PALM-4U, not PALM (Sect.2.1 and Fig. 1). However, in Sect. 2.5.5, it seems that the chemistry module was with PALM, and PALM-4U was not appeared. In Sect. 2.5.6 as well. It is a bit confusing. Please clarify the relationship or difference between the two models and be accurate in the definition throughout the manuscript.
Author's resp: PALM is primarily an LES code with an additional RANS mode. The PALM model comprised of a dynamic core and various embedded models. PALM-4U is the conceptual framework of the model components embedded/coupled to PALM which are specifically designed and/or used for urban applications. The description of PALM and PALM-4U has been rephrased in the text (abstract and in section 2.1) so that to make the difference more clear and easy to understand (Pg 1, Ln 4-5; Pg 4, Ln 21-23).
"... The new chemistry model is implemented in the PALM model as part of the PALM-4U components (read: PALM for you; PALM for urban applications) which are designed for application of PALM model in the urban environment (Maronga et al., 2020)..."

Subsection 2.5.5 and 2.5.6 does not exist in the manuscript, therefore, the issue raised by the reviewer cannot be addressed.

Comment(5) P.4 Ln. 16: "Optical cloud and rain water" may require explanation. It was written later that cloud microphysics was not implemented, so what are they?
Author's resp: We never wrote that cloud microphysics was not implemented. Since PALM version 4.0 a bulk liquid-phase two-moment microphysics scheme is available which predicts rain droplet number concentration and rain water mixing ratio. To avoid any confusion, the text has been slightly rephrased (Pg 4, Ln 24-26).
" ... the three velocity components (u, v, w) on staggered Arakawa C grid, and four

scalar variables namely potential temperature (θ) , water vapour mixing ratio (qv), a passive scalar s and the subgrid-scale turbulent kinetic energy (SGS-TKE) e (in LES mode) (Maronga et al., 2019, 2020)..."

Comment(6) Figure 1: Arrows are ambiguous. What's the difference between grey arrow and green arrows? What's the difference between the green arrow with single direction and bi-direction? It seems that emission to chemistry driver is one-way, but there is a direction from chemistry toward emission. What process is it?
Author's resp: Green and thick grey arrows were added to improve presentation of the flow chart. However, to avoid any confusion, all arrows are now drawn in grey colour. The thin arrows show the general flow and direction of the data within the Chemistry model and its components whereas thick grey arrow indicates coupling of the Chemistry driver with the PALM model core (Pg 5). Figure 1 is uploaded for review.

Comment(7) P.6, L.15 "deposition, scavenging" -> "deposition and scavenging"
Author's resp: The text is updated (Pg 6, Ln 15).
".... (i.e. deposition and scavenging)."

Comment(8) P.8, L.13 "Fast-J" may need reference. If it is an abbreviation, please spell it out.
Author's resp: The text is updated and an appropriate reference Wild et al. (2000), has been added (Pg 8, Ln 5-6).
"... More extensive photolysis schemes such as the Fast-J photolysis scheme (Wild et al., 2000) that are based on the radiative transfer modelling will be included in the future..."

Comment(9) P.8, L.20-21; for aerosol phase, better to write sulfate (SO42-), nitrate

(NO3-), and ammonium (NH4+).
Author's resp: The text has been updated (Pg 8, Ln 13-14).
"... 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) ..."

Comment(10) P.9, L.10: "following (Simpson et al., 2003)." -> "following Simpson et al. (2013)."
Author's resp: The reference has been updated (Pg 9, Ln 12).
" ... calculated following Simpson et al. (2003)... "

Comment(11) P.9, L.29: "The chemistry model of PALM" -> "The chemistry model of PALM-4U", right?
Author's resp: Yes, this is right. the text has been updated (Pg 9, Ln 30).
"... The chemistry model of PALM-4U includes a module for reading ..."

Comment(12) P. 10, L.12 "modes": "sectors" are more frequently used. Please consider to rephrase.
Author's resp: Thanks to point this out. We agree this sentence was slightly misleading. We have rephrased and improved the text (Pg 10, Ln 11-13).
"... More detailed traffic emission data can be provided in gridded form in PALM-specific NetCDF files (Maronga et al., 2020). LOD 1 emissions are gridded annual emission data for each sector (e.g. industry, domestic heating, traffic), which will be temporally disaggregated using sector-specific standard time factors..."

Comment(13) Sect. 3.1 "numerical set-up" includes several sentences which should be described in different sections.

a) P. 11, L. 2: "Details of the dynamics core ... Maronga et al. (2020)" better to be moved to a model description section, Sect. 2.x.
b) 2nd paragraph of Sect. 3.1, the first two sentences "Observations from ... a 24 hour run." and "The ceilometer observations ... the diurnal cycle" and the latter two sentences "Fig. 2 shows ..." and "The horizontal grid spacing..." are not relating with each other. The description of weather by Ceilometer observation was already mentioned in the 1st paragraph of Sect. 3.1. Better to reorganise the 1st and 2nd paragraph of Sect. 3.1.
c) P. 11, L. 26, "A third order Runge-Kutta, ... (Wicker and Skamarock, 2002)" are already written previously.
Author's resp: a) "Details of the dynamic core ....", has been moved to model description section 2.1 (Pg 4, Ln 32-33).
b) 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 –).
c) This is probably fine. The first time Runge-Kutta and Wicker and Skamarock appeared in the general model description while on the second time, both appeared specifically as part of the model setup for simulations.

Comment(14) P. 11, L.12: Spell "TU" out here.
Author's resp: The abbreviation (TU) is removed and the actual name "Technical University" has been used instead (Pg 12, Ln 13). "... Charlottenburg building of the Technical University of Berlin ..."

Comment(15) P.11, L.165: "Ceilometere" -> "Ceilometer"
Author's resp: The spelling has been corrected (Pg 12, Ln 18).

Comment(16) P. 12, L. 2: Probably "(Resler et al., 2017; Maronga et al. 2020)" looks

better.
Author's resp: Both of the citations have been updated in the text (Pg 13, Ln 18).
"... the urban-surface model (Resler et al., 2017; Maronga et al., 2020)."

Comment(17) P. 12, L.16: "Monin-Obukhov Similarity Theory (MOST)" mentioned already several times in the previous locations. Define MOST when it is first appeared and use MOST in the following locations.
Author's resp: The Monin-obukhov similarity theory is abbreviated as MOST, the first time it appeared in the text, and then only "MOST" used in the following text (Pg 4, Ln 28).

Comment(18) P.13, L.25-35: How the authors set the boundary conditions for chemical species are not explained.
Author's resp: The description of the chemical boundary conditions on lateral, top and bottom boundaries has been further improved to make it more clear and easy to understand (Pg 14 Ln 19-20; Pg 14, Ln 29-31).
"... At the bottom boundary, a Dirichlet condition is applied to flow, θ, and q whereas a Neumann condition is applied to e, p and chemical compounds. Moreover, a canopy drag coefficient C_d = 0.3 has been applied while the roughness is specified internally depending on vegetation type. At the top boundary, Dirichlet boundary conditions are applied to flow and and p only, initial gradient is applied to θ while Neumann boundary conditions are applied to q and chemical compounds..."

Comment(19) Sect. 3.2: Please provide the heights of the observation sites, Wedding and Hardenbergplatz. In urban locations, the observation points could be on the roof of building. If this is the case, comparison between the simulated 5-m height concentration and the observed roof-top concentration are inconsistent.
Author's resp: The average height of air quality sensors is around 4 m above ground.

Therefore, comparison between observations and model data which is extracted 5 m above ground is consistent. The text has been updated in section 3.2 (Pg 12, Ln 26). "... average height of the air quality sensors at both stations is 4 m above ground..."

Comment(20) Sect. 4.2: The chemistry module and the grid point used to depict Fig. 4 was missing. Probably CBM4 and Hardenbergplatz, though.
Author's resp:: These are the spatial mean profiles of concentration and fluxes. The text and figure caption has been updated by adding "mean" and "simulated with CBM4 mechanism" (Pg 15, Ln 17; Pg 16, Ln–).
"Figure 3.Vertical profiles of a) potential temperature, b) mixing ratio, c) wind speed and d) wind direction, at different times from morning to midnight on 17 July 2017. The horizontal bars in a) indicate the boundary-layer height derived from ceilometer observations."
"... Figure 4 shows mean profiles of concentrations and vertical fluxes of NO, NO2, O3and CO for the selected times of the diurnal cycle on 17 July 2017, simulated with the CBM4 mechanism..."

Comment(21) P. 24, L. 5: "Figure 10" -> "Fig. 10"
Author's resp: The inconsistency in the use of '$Figure$', and '$Fig.$', has been removed. In the beginning of the sentence we use '$Figure$', whereas within the sentence we use '$Fig.$'. The use of both is now consistent throughout the manuscript.

Comment(22) Table 2: It is quite reasonable that the CPU time of transport only without meteorology of CBM4 was 10 times that of PHSTAT (310/30) because the number of tracers is also 10 times (32/3). However, with chemical reactions, why the CPU time of CBM4 was still 10 times that of PHSTAT (550/50) even though the number of chemical reactions of CBM4 (81) is 40 times that of PHSTAT (2). Is it because only two reactions with KPP requires as much CPU time as 81 reactions?

Author's resp: It is correct that CBM4 is 10 times more expensive than PHSTAT both for 'transport-only' and for 'Full' (transport + reactions) simulations. The relative increase of the computational expense for the solution of the chemistry equations does indeed decrease with increasing number of chemical compounds. As explained in section 3.4 of Verwer et al. (1999), the efficiency of the applied Rosenbrock solver increases with increasing size of the chemical mechanism. A corresponding sentence was added to the text (Pg 27, Ln 17-24).
"... The results show a significant increase in the computational cost relative to the meteorology only simulation for the same model domain. The comparison of 'transp. only' and '(full)' for Case A (Table 2) shows that the transport of additional scalar variables is even more expensive compared to the computation of the chemical transformation. While the increase in computational costs for the transport increases linearly with the number of compounds, this is not the case for computation of chemical conversion. As described by Verwer et al. (1999) the efficiency of the applied Rosenbrock solver increases fortunately with increasing size of the chemical mechanism. Comparison of 'transp. only' of case B with 'full' suggests that for the PHSTAT mechanism the computational expense for the transport of the additional scalars is almost the same as for the computation of the chemical transformation..."

Comment(23) Overall, the authors show horizontal variations in concentrations in Figs. 8 and 10 and vertical profiles from 0 m to 2,500 m in Figs. 3, 4, 5, and 9. However, they did not show the vertical profiles in the bottom layers (i.e., below 50 – 100 m), even though there seems very sharp vertical gradients. This might be of interest. Is it possible for the authors to show the horizontal distributions of concentrations near the top of urban canopy (at several ten meters?) to compare and discuss the differences from those at 5 m of Fig. 6, for example? Large scale models can only simulate the concentration above the urban canopy and many of the urban observation points exist on the roof of buildings. It is very informative for large scale modellers to show the difference in concentrations between the street canyon and urban canopy top.

Author's resp: In figure 3 and 4, vertical profiles of meteorology, pollutant concentration and pollutant fluxes are provided from surface to 3 kilometre above ground. Sufficient explanation of these profiles is already provided in the text. However, a detailed analysis of the urban canopy processes is out of the scope of this paper.

References

Verwer, W G., Spee, E J., Blom, J G., Hundsdorfer, W., 1999:A second order Rosenbrock method applied the photochenmical dispersion problems.*Journal of Atmospheric Chemistry*,**37**,. doi:10.1137/S1064827597326651.

Wild, O., Zhu, X., Prather, M. J., 2000:Fast-J: Accurate Simulation of In- and Below-Cloud Photolysis in Tropospheric Chemical Models.*IAM Journal on Scientific Computing*,**20**, 1456-1480. doi:10.1023/A:1006415919030.