Geosci. Model Dev. Discuss.,
https://doi.org/10.5194/gmd-2020-286-RC1, 2020

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.

Anonymous Referee #1

Received and published: 11 November 2020

Recommendation: Minor revision

General comments:

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.

Specific comments:

(1) The country names are missing in the affiliations of co-authors from #2 to #6.

(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.

(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.

(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.

(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?

(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?

(7) P.6, L.15 "deposition, scavenging" -> "deposition and scavenging"

(8) P.8, L.13 "Fast-J" may need reference. If it is an abbreviation, please spell it out.

(9) P.8, L.20-21; for aerosol phase, better to write sulfate (SO42-), nitrate (NO3-), and ammonium (NH4+).

(10) P.9, L.10: “following (Simpson et al., 2003).” -> “following Simpson et al. (2013).”

(11) P.9, L.29: “The chemistry model of PALM” -> “The chemistry model of PALM-4U”, right?

(12) P. 10, L.12 “modes”: “sectors” are more frequently used. Please consider to rephrase.

(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 reorganize 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.

(14) P. 11, L.12: Spell “TU” out here.

(15) P.11, L.165: “Ceilometere” -> “Ceilometer”

(16) P. 12, L. 2: Probably “(Resler et al., 2017; Maronga et al. 2020)” looks better.

(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.

(18) P.13, L.25-35: How the authors set the boundary conditions for chemical species are not explained.

(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.

(20) Sect. 4.2: The chemistry module and the grid point used to depict Fig. 4 was missing. Probably CBM4 and Hardenbergplatz, though.

(21) P. 24, L. 5: “Figure 10” -> “Fig. 10”

(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?

(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 modelers to show the difference in concentrations between the street canyon and urban canopy top.

Interactive comment on Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2020-286, 2020.