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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Impacts of physical parametrization on prediction of ethane concentrations for oil and gas emissions" *by* Maryam Abdi-Oskouei et al.

Anonymous Referee #1

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Review on: "Impacts of physical parametrizations on prediction of ethane concentrations for oil and gas emissions" by Maryam Abdi-Oskouei et al.

In this article the authors test the influence of different configuration of the WRF-Chem model on the modeled ethane concentration. More specifically, they test three boundary layer schemes, two different dynamical boundary conditions, a scaling of the emission inventory, the effect of a free running simulation versus a re-initialised one and the impact of the horizontal resolution (12 km vs. 4 km). Investigation of the influence of different model configurations on the simulation results is an important issue, specifi-

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Discussion paper

cially for chemistry simulations where ensemble simulations can not be performed due to limitations in computing power and storage space. Unfortunately, the article stays at the surface of such investigations, solely comparing the differences of the simulations. Neither the authors go into the detail where these differences come from, nor do they draw any conclusions on the configuration, which should be chosen in future simulations.

This article requires at least major revisions. From my point of view a re-submission after a thorough revision would be the better way, as the article needs to provide much more substantial information to the reader.

The following points are ordered by appearance in the article, not by importance:

Major points:

Sect. 2.2:

- With the horizontal resolution of 4 km x 4 km the smaller domain is well within the gap between the horizontal resolution where convection parametrisations are fully applicable and the convection resolving scale. The information, which convection parametrisations are still active in the 4 km domain (all or only deep convection) needs to be added to the model description. Note, that the influence of the choice of the convection parametrisation on the simulation result needs to be discussed (at least in the section where the influence of the horizontal resolution is investigated).
- Many informations on the chemical initial and boundary conditions (IC/BC) is missing: In which time interval are new BC data applied? Are the IC/BC data provided for this specific time interval/date? If yes, how do they fit to the two different dynamical boundary conditions used?
- How many species are included in the used chemical mechanism?

Sect. 3.:

- The title of the section is wrong. So far it provides only a listing of differences between the sensitivity simulations (results), but almost always neither an explanation for the differences is provided, nor is discussed, what the consequences for future simulations are (discussion).

- Use of the supplement for figures and tables:
  All in all I very much appreciate to provide additional information in the supplement. Anyhow, in your case I got the feeling that the article should be shortend by putting tables important for the discussion into the supplement, while desirable extra information which would be well suited for the supplement is missing. More precise:

  - Table SM4 (maybe SM3) should become part of the main paper.
  - Figure 2 might provide a nice overview over all simulations, but it does not provide enough information for the comparison of the respective sensitivity simlations. Simply because of the number of lines (different symbols) not all simulations are identifyable. Here the supplement could be used to provide a figure 2 like figure individually for each of the tested parametrisations (one for the PBL schemes, one for (re-)init, one for IC/BC, one for horizontal resolutions and on for the different emission scenarios).
  - Figures SM1 / SM2: some as for Fig. 2 add individual panels for those comparisons referring to SM2 (PBL and re-init). Maybe add reference to SM 2 also for the other tested parametrisations?
  - Figure 3 and Figure 4: Same as for Fig. 2. Use the supplement to provide the plots individually for each sensitivity study, where the lines are hardly distinguishable otherwise.
  - Figure 3/4: dashed and solid lines are not distinguishable in the legend.

- Why are the tables for the model performance only provided for BAO station? It would be nice to be able to compare the so far provided statistics to the other stations listed in the introduction.
- Tab. (4 / SM3 / SM4) (3 / SM2) Why do you show observations in a row? In this way you have to repeat the value for the observations for each simulation. Just show obs in an additional column! In this way you could easily combine Tables 4, SM 3 and SM 4 and Tables 3 and SM 2 in one landscape table, respectively.

- p. 7, 26./27.: Here I disagree, not “all” simulations show better skill at daytime. Better change “all simulations” to “most simulations”.

- p.8, l. 15 / l. 29: I am missing any information why the AM and PM flights are different and any suggestions, why the modeled concentrations are off by such a hugh amount. If these points would be sufficiently discussed in the following subsections, it would be ok to refer to the following analysis, but so far, they are not discussed in the further analysis either.

- Sect. 3.1:
  - as already mentioned,the difference between the PBL simulations hardly visible in Fig. 2. It would be good to have a figure showing only the three simulations and the observations in the supplement.
  - Why do you use different chemical initial and boundary conditions for the PBL sensitivity studies (MACC) in contrast to all other sensitivity studies (Table 2)? This courses additional differences you never discuss.
  - p.9, l.16: Cite Figure SM1.
  - Fig. 6: Article Text states “Fort-Collins-West (FCW)” , figure shows “FT”.
  - p.9, l.26: For a non-specialist for boundary height measurements: Why is a quantitative comparison not possible?

- end of section: What are the consequences? Does the choice of PBL scheme matter or not? Which PBL scheme will you pick in future?

- Sect. 3.2:
  - You change here from simulations driven by NCEP and MACC data, to simulations driven by ERAinterm and RAQMS data. Some information, why not the same driving data is used is missing here.
  - p.10, l.28.: "in addition, Init 4 predicted higher wind speeds compared to Init5." And compared to Observations?
  - p.10, l.28.: Any suggestion, which simulation is more realistic?
  - p.10, l. 30/31 and 34 : Why does Init4 show the by far lowest ethane concentrations for C130-AM and all P3 flights? I thought the chemistry is not re-initialised in the same way as the meteorology?

- Sect. 3.3:
  - The evaluation how much the simulation changes with respect to the meteorological initial and boundary data is meaningless without a comparison of the differences in the driving data themselves. How close are the reanalyses of ERA-Interim and NCEP-NFL to the observations in the area of interest?
  - p. 11, l. 7-9: as far as I can deduce the correct lines from Fig. 2 and SM 1, both simulations overestimate temperature and underestimate moisture, where the ERA-Interim simulations is more off than the NCEP simulation.
  - p.11, l. 14/15: I do not understand, I thought the Denver cyclone was not part of the analysis (top page 7). If this is just another "feature" and not the explanation of the huge differences in Met6 simulation for P3-PAO add this explanation and indicate by a line break, that you are talking about something new.

- p. 11, l.19/20: Why do the simulations miss the event?
- p. 11, l.22 / SM4: Please show the absolute values (at least of one of the simulations) as well, otherwise absolute differences do not provide the full picture. This Figure should be part of the main paper. If you want to discuss the Denver cyclone, figure SM4 should be part of the main paper. But in this case, the analyses should go beyond the mere stating of the differences.

Sect. 3.4:

- p. 11, l. 27: No, the domains are not run "independently" as the 4x4 km^2 domain depends on the 12x12 km^2 domain.
- p.11, l. 28./29.: What about temperature and relative humidity at PAO and WC tower?
- p. 11, l. 28 /31: The different labels are hard to detect in the Figure 2 / SM2.
- p. 11, l. 31. This is only true at nighttime (Tab. 4 / SM 4). Cite the tables in the text.

Sect. 3.5:

- p. 12, l. 16: According to caption, Fig. 8 shows measurements. How can it be seen, that the model does not match the measurements? This is seen from Fig. SM 5, therefore this figure belongs in the article, not in the supplement. The phrase "as shown in Fig. 8a" is very irritating. It belongs in front of the "which", i.e., after the statement about high values of ethane.
- as the comparison of the two emission scenarios is the topic of this subsection, SM 6 also belongs into the main paper. However, Fig. 9 could be part of the Supplement.
- p.13, l.18/19: I do not think that you need an indicator for low emission rates. These are input by the emission inventory, thus this is aprior knowledge.

  - Discussion of Fig. 10: Say more about the best fit lines (meaning of differences in intercepts and slope).
  - p. 13, l. 31/32: Where do I see these low biases (cite respective table / figure)

- What about cross evaluation? What changes with different chemical IC/BC? What is the influence of the PBL scheme for the higher emission szenario?

Conclusions:

- p. 14, l.10-22: In this section "NMB" and "NMB variability" is falsely used synonymously. It might be true that the inter-simulation variability of NMB might be usable "as a proxy for variability in the model performance caused by model configuration". But the percentages listed below are only the NMBs and not the inter-simulation variability of the NMB.
  However, this paragraph again only lists (new) results (not even a discussion). Therefore it does not belong in the conclusion section.

- p. 14, l. 24 - p.15, l. 4: This section stays very in-concrete. All the species discussed here have a medium range lifetime. Nevertheless, the aspect of the influence of chemical initial and boundary conditions is completely left out.

- For me the final conclusion is missing: Based on this study, what has to be taken into account by setting up a WRF-Chem simulation? What would be the best WRF-Chem setup?

Minor points:

- From my point of view WRF-Chem is not a Chemical Transport Model (CTM). The term "transport" includes the fact, that the chemical substances are transported,

but they do not feed back to the dynamics. WRF-Chem is a fully featured regional atmospheric chemistry model (RACM) which very well includes e.g., radiation and cloud feedback. Therefore I recommend to omit the term CTM with respect to WRF-Chem. I know that whole communities use this term wrongly, but this did not change the misconception of it.

- As this article is very WRF-Chem specific, it would be apropriate to name the model in the title of the article, e.g. “Impacts of physical parametrizations on prediction of ethane concentrations for oil and gas emissions a case study with WRF-Chem v3.6.1” or ‘Impacts of physical parametrizations of WRF-Chem (v3.6.1) on prediction of ethane concentrations for oil and gas emissions”
- Sect. 2.3: Add more information on how the emissions of 76 species are mapped to the species of the chemical mechanism used.
- p.7, ll. 5-17: add the information, that these results will be discussed in more detail in the following subsections.
- p.7, ll. 19-34: add the information, that these results will be discussed in more detail in the following subsections.
- p. 10, l. 10: cite Table 5.
- p. 10, l. 11: cite Fig. 4.
- S1: Sums over i without any “i”s in the equations? What is “n”? IOA is introduced (also in the article) but never referenced.

Typos & Co:

- p.4, l. 26: remove “Tables and Figures”

- p.5, l. 8: Did you consciously choose an abbreviation (4-MnERi) which is not included in Table 2 ?
- p.5, l. 9: The abbreviation of the PBL scheme is (MYNN3)
- Through out the article (and in the figures) inconsistent abbreviations for Fort-Collings West are used (FC, FCW ...). This should be uniform.
- Fig. 5: What is the meaning of the line at 41 N ?
- p. 9. l. 11: Cite SM 3/4 at end of sentence.
- p. 9. l. 11: Fig. 5 does not “compare” anything, it “visualises”, “shows”, “depicts” ...
- p. 9, l. 30 / 31: use full sentences: “PBL1, non-local PBL scheme” → “ PBL1 using a non-local PBL scheme”.
- p. 11. l. 20: A figure does not “compare” anything, it “visualises”, “shows”, “depicts” ...
- p. 12, l. 14, Fig. 8: Limited to 200agl or 1500 m ?
- Fig. 8.: If these are measurements, what does “grids with more than 4 measurement points” mean?
- Fig. 10: Improve caption. The second sentence sound as if model vs. measurements are plotted.
- Fig. 10 / 9: give parameters of best fit line.
- Tab. 5: Is the NMB for PBL3 P3-BAO really 0 ?
- SM2: caption: state that “surface winds” are shown.

- Table SM4: omit line breaks for init5
- Fig. SM3: What is surface ethane: ethane in the lowest model layer?

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