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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 #2

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The manuscript 'Impacts of physical parametrisation on prediction of ethane concentrations for oil and gas emissions' by Maryam Abdi-Oskouei and co-authors describes a model sensitivity study applying WRF-CHEM to air pollutant simulations in the Denver, Colorado, area. The study focuses on the effect on tracer transport related to oil and gas extraction. The manuscript is well written and overall well structured. For the most part, the applied methods are appropriate and constructive. However, some additional clarifications concerning the aim of study and the drawn conclusions are required before the manuscript can be published.

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Discussion paper

Major comments

Aim, approach and conclusions: The aims of the presented study are somewhat twofold. 1) evaluate the chemistry-transport model and 2) draw some preliminary conclusions on the emissions from oil and gas extraction in the Northern Front Range Metropolitan area (NFRMA). In general, I agree with the authors that a transport model needs to be validated before it can be used for inverse modelling purposes (here emission estimation). However, these two subjects are somewhat mixed together in the study, since one main evaluation parameter of the model system is the ethane concentration, which strongly depends on the emissions, which one finally would like to determine. The manuscript would gain in significance if these two subjects (transport model performance and emissions from oil and gas) could be separated more more clearly in the presentation of the results. Instead of evaluating model performance for ethane another model tracer (e.g. carbon monoxide) should be given more attention during the evaluation part of the manuscript. Since carbon monoxide is largely unrelated to the oil and gas emissions and its emissions are otherwise relatively well know, one should be able to distinguish, which model configuration is best suited for tracer transport simulations. Only afterwards, the less well known ethane emissions should be discussed.

In this context another question arises concerning the application of the full chemistry version of WRF-CHEM in the sensitivity runs. A passive tracer setup (as available in WRF-CHEM) would have been sufficient to carry out the sensitivity runs as well. Only the discussion including shorter lived VOCs really grants running the complete model. This is more a comment for future sensitivity simulations than for the current manuscript. However, since the complete chemistry model was run, it would also be interesting to have a look at a secondary pollutant (e.g., ozone) and how it reacts to the emission variations in the final sensitivity experiments. Most likely ozone observations were available from all flight campaigns and additionally surface sites. The model-

observation mismatch for ozone might deliver another hint towards the suspected underestimation of emissions from gas and oil extraction.

Finally and coming back to the beginning, the conclusions of the paper should give more emphasise to the finally selected model configuration. Which is the best configuration, which parameters were most important to change, and why does the change make sense? Without such a recommendation (although not necessarily valid for other study areas or periods) the whole presentation of sensitivity results remains of no avail for the reader who wants to find concrete hints for setting up his/her own simulations. Right now the conclusion only summarises all sensitivity simulations together, although there were clear performance difference for some of the runs (PBL1 vs PBL3, free-run vs re-ini, etc). These are important details of the model setup that should be more easily accessible when browsing the paper.

Minor comments

Page 2, Line 9: From the context and my own knowledge of emissions from the oil and gas sector it remains unclear why NOx emissions should play a major role in the extraction process. Is it due to fossil-fuel operated machinery (compressors, pumps, etc) or due to flaring? In the discussion of the model results there is no more mentioning of NOx either. Was it not observed on-board the aircraft?

P3, first paragraph: Others have used WRF-CHEM already for 'inverse modelling' of emissions from oil and gas extraction. The study by Barkley et al. (2017), which used WRF-CHEM for CH4 emission estimation (although not with full chemistry), should be mentioned as well. Either when mass balance approaches to estimate emissions are discussed or more general in the discussion of the results.

Subsection 2.1: The presentation of the observations is lacking any reference to the applied measurement techniques, data quality, etc. Some of this information is given

later when the results are presented, but it should actually be presented in this subsection. For the more involved measurements (VOC concentrations) it would also be nice to learn a bit about observation uncertainties before comparing with model results.

P4,L30: The kind of VOC lumping used in RACM should be mentioned. Is ethane treated explicitly? How many chemical species are present?

P5,L21 and elsewhere: Since it was mentioned above (P5,L10) that the simulation ID according to table 2 would be used throughout the text to identify the sensitivity simulations, I see no need to give the simulation name here as well. All these abbreviations will only confuse. All figures also contain a mix of names and identifiers that are not according to the ID. This should be unified, so that the reader only has to follow one set of abbreviations.

P6, 1st paragraph: What is the rational for this re-initialisation? The model domain is relatively small. Shouldn't the BCs dominate anyway? In this context it should also be mentioned why no meteorological data assimilation was run for WRF, which probably would have reduced the spread in the sensitivity tests significantly.

P7, L5: 'average error'. Should this be absolute error, which would actually fit the definition in the supplement.

P7, L6: Although the supplement provides the definition of the comparison parameter 'index of agreement', it would be nice to give a short interpretation of its benefits and expected value range for a well performing simulation. Furthermore, values of IOA are presented in a table, but never discussed in the text. Something that is true for other comparison parameters as well. If they are shown in the table a short description and interpretation in the text should also be given.

P7, L9: I feel like one could start a new subsection here (after 'model values') that deals with the general results. Everything before is an introduction to the results, now the first real results are shown.

P7, L25: Maybe I missed this somewhere else, but at which altitude were the measurements at WC tower and PAO taken?

P8, L12 and elsewhere in manuscript: Values of NMB are discussed. But are they shown anywhere in the tables or figures? If yes a cross-reference to the figure would be useful, if not this should also be mentioned (e.g. adding 'not shown'). Otherwise the reader will try to confirm this information in one of the figures.

P8, L31ff: It is argued that the model 'represents the profile shape [...] well.' I don't agree with this completely and for all cases. For the afternoon observations, where C130 and BAO observations actually show relatively low values at the bottom of the profile, most model runs still show a smoothly increasing concentration towards the surface. What is the potential reason for the observed profile shapes and what does the model miss here?

P9, L26: It is argued that a 'quantitative comparison between model and measurement [of PBLH] is not possible'. I don't agree. It depends on the situation, but during the day the agreement between a lidar-derived PBLH and one derived from temperature profiles should actually be pretty good as long as you have an aerosol-laden PBL, which is most likely the case in the American South-West. See also Collaud Coen et al. (2014).

Figure6: I suggest to extend this figure for all other sensitivity simulations as well. Next to wind speed, PBLH is the most important dispersion parameter on local to regional scale. The use of the same turbulence scheme in all other sensitivity runs will not necessarily lead to the same PBL heights. For example the two different BC runs are also likely to result in different PBL structures.

P10,L7ff: This paragraph should include a short description of the changes in profile shape for the different PBL runs. The interesting part is that with PBL2 and PBL3 and although these runs are supposed to produce more realistic PBL heights, the increase in PBL concentrations compared to PBL1 is opposite to what the observations suggest

(Fig 3 and 4). That is: afternoon concentrations increased from PBL1 to PBL2 and PBLE3 below a certain altitude, but the resulting profile shape is then even less in line with the observations.

P11,L14ff: In the beginning of the results section it is mentioned that the Denver cyclone period was removed from the analysis. Why is it presented here again? Either this part should be moved to the beginning of the results section when justifying why the phase was excluded from the analysis or it should be mentioned here again which period is really contained in the figures.

Section 3.5: Megan biogenic emissions are mentioned in the Table but not in the text. What is their significance for this sensitivity run and overall for this study? Did Megan predict significant emissions of ethane or HC3? Probably not!

P12,L27f: Not surprisingly, the measurements did not differ for the two different simulations! Should it be 'simulated CO'?

P13,L21ff: In the discussion of Figure 10 it should be mentioned that for the longer-lived HC3 one should/could have removed a background concentration. The presentation is still valid if only the slopes/ratios are discussed and background did not change over the domain of interest. The latter should be commented on.

P13,L26f: Following up on the last comment, it most likely is not recently emitted HC3 that leads to elevated levels but background levels. The alkanes contributing to HC3 are relatively long-lived and the HC3 concentration at the domain boundaries is most likely a few ppb. This could be easily checked in the model fields. In contrast TOL is relatively short-lived, so BC concentration are probably close to zero.

Technical comments

P2,L25: 'Thousand Cubic Feet' probably supposed to be 'Million Cubic Feet'. Also, I

am not sure if ACP allows US customary units.

P9,L22 and elsewhere: 'Fried, 2000' is not the correct formatting. Please refer to the ACP guidelines.

References

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