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Atmospheric Chemistry and Physics Discussions

Interactive comment on "A chemical transport model study of plume rise and particle size distribution for the Athabasca oil sands" *by* Ayodeji Akingunola et al.

Anonymous Referee

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This discussion paper presents results of simulations with the operational Canadian chemistry-transport model GEM-MACH. A range of different model and input options is tested and compared with surface and aircraft measurements in the Alberta oil sands region. These options consist of different aerosol size resolution, different plume-rise formulations, and different data for the stack emission parameters. The authors found that using twelve instead of two aerosol size bins reduces the model bias for PM significantly. For the plume rise formulation, the results are less clear and the authors question whether improvements come for the right reasons. Real hourly stack data did not improve the results, and the question why remains unanswered.

This paper introduces a very interesting and potentially highly useful field campaign. It also provides important insights into the performance of the operational Canadian model. However, the paper has some weaknesses listed below.

1. In the same special issue for which this paper is submitted, there is another paper by the same group of authors, Gordon et al. 2018, which is also devoted to the plume rise topic, and it is said to have found opposite results. Neither is the reason for that clearly resolved, nor does it become clear why the plume rise topic is split between two papers.
2. The model performance is not only influenced by the aspects forming the focus of this paper, but also by the accuracy of the meteorological part of the model, and by the numerics of transport, notably the vertical diffusion and the handling of the point sources in the Eulerian framework. Their role is discussed only at the very end and, in my opinion, not sufficently in depth. In order to evaluate specific model aspects, one first needs to understand the performance of the model in general, with its strengths and weaknesses.
3. The statistical approach chosen for the evaluation of the model options relies on metrics which exclusively are based on "match in time and space" data pairs. It is well known in air-pollution modelling that for near-source conditions (which is what we find here), there is often too much "noise" in the data (be it due to the stochastic nature of the plume, be it due to unresolved meteorological variability) to give meaningful results. Correspondingly, some of the statistical parameters are not very good. Therefore, global comparisons (such as deviations from the cumulative frequency distribution, statistics of cross-wind integrated values, or average dependency on key parameters such as stability and wind speed) are often used to assess models in a more robust way.
4. The paper is written well on the "small scale" (apart from numerous technical deficiences as listed below), but the broad topics could be worked out more clearly.

In the end, the findings are: twelve aerosol size bins are better than two (not surprising, but good to see it quantified), there is an improvement by using the model's vertical profile information for plume rise calculation but given the model's deficiencies the overall conclusion seems to be not so clear, and no improvement was found for using hourly stack data, but it remains unresolved why. We may wonder whether the work is mature enough for publication if we consider this state of the quintessential findings.

Specific comments

1. Page 2, l. 18: Why are you thinking that reasons for weak performance include only those meteorological variables that are used for the plume rise calculation, but not, for example, wind direction?

2. The model overview section lacks information on the numerical scheme used for vertical diffusion even though this is crucial in the context of study (cf. discussion on p. 24). The main reference for the MACH model seems to be Makar et al. (2010) – an extended abstract that would not be available for most people who haven't attended the conference as it is not freely accessible. Is there no more detailed and open description of this model? Note that also the Coté et al. citation is one of those for which the reference is missing. In addition, the handling of the point sources is not described (usually, Eulerian models use some sub-model to track plumes until they match the size of the grid cells).

3. The model set-up description in section 2.2 is not easy to follow. It might be helpful to move some of the information into a table and to shorten the text.

4. Page 8, line 1: The plume's buoyancy flux is **not** dependent on the stack height (at least not directly).

5. From the sentence beginning on p. 11, l. 7, on, the text does not really belong to the section 2.2.3. It should become a section of its own, as it introduces the simulations forming the base of the rest of the paper (maybe merge with some parts of the 2.2 chapeau).

6. Page 11, Section 3.1: What is the justification for removing measurements with values exceeding some threshold? Without proper justification this would not be acceptable.

7. Page 12, Section 3.2: The phrase 'spatial linearly interpolated model values at the models chemistry time resolution of 2 minutes' is awkward. If you have 10 s data as said before, why do you need to interpolate for obtaining 2 min data? Also, it would be good to know which distance corresponds to both 10 s and 2 min flight data, and how this compares to the model's grid size.

8. Section 4 (Results and Discussion) needs to be structured into subsections.

9. Table 1: Apart from widely used or self-explanatory metrics such as FAC2, RMSE or r, the metrics parameters need to be defined.

10. Page 12, l. 31: "Figure 2 shows that the model simulations are biased high for particles less than 5 μm diameter, and biased low for the larger particle sizes." As this figure only shows results for PM2.5, a statement on larger particles can't be based on it.

11. Page 13, l. 14: Information on the bin sizes belongs to the model description section, not the result section.

12. Page 13: The second paragraph on this page contains a number of statements about results without pointing to the figures or tables which show them.

13. Concerning the model performance for PM, it should be discussed that even though the twelve-bin version leads to significant improvements, major discrepancies to observations remain.

14. A number of tables are presented where several metrics are used to compare various model versions, with the best one being emphasised by bold print. Sometimes, differences are tiny and probably insignificant. Only those values that are *significantly* better should be highlighted to avoid a wrong impression of the results (for example, in Table 3 the model version seems to have no impact for O_3 but we get the impression that the simpler model is better.)

15. Why is the use of hourly emission data beneficial for NO_2 but detrimental for SO_2?

16. The discussion paper does not comply with the ACP Data Policy; it does not have a "Data availability" section and says nothing about data availability.

Technical comments

In this manuscript, there are many details that need to be corrected or improved. I hope that I have identified most of them, nevertheless I would call upon the authors to generally pay more attention to those details in their revised manuscript.

The following list mentions such topics either globally or, for some, individually.

1. Page 2, l. 14: CEMS has nothing to do with observations.

2. Spelling mistakes that are not caught by a spell checker. I noticed for example "RAND" instead of "RANS" on page 3, line 11, but there may be more. Please proofread your manuscript.

3. Page 3, line 11ff.: This sentence is a bit awkward, rephrase it.

4. Writing of numbers with units: don't forget to leave a (at least thin) space between them.

5. Punctuation: There are instances of doubled or missing punctuation, or inappropriate use of the hyphen.

6. Write out numbers from one to twelve if they occur in the running text.

7. Page 3, l. 22, "lower values" would fit better here than "lower elevations" (elevation refers to topography).

8. Page 4, l. 8: Create a proper reference for SMOKE instead of putting it into the text.

9. Page 5, l. 5: "data-assimilated meteorological analyses" is not proper English.

10. Fig 1: Do not confuse the indication of subfigures with the indication of domains in the first subfigure. Due to the dark background, subfigures d) and e) are not readable. It might be better to show topography or land-use in a simple way rather than a satellite image. Why do they show two different domains? Also, I don't understand what "Google-Earh-referenced" means.

11. On page 8, please pay attention to how you incorporate the equations into the surrounding text (what is a full sentence?)

12. Case distinction for Eqs. 2, 3, 4: While the conditions are correctly formulated, they might be easier to grasp if they were expressed in terms of h_s instead of L, adding a second condition (with the sign of L).

13. Page 8: I have not compared these (or other) equations with the original source (Briggs), but given the number of typos in this manuscript I would recommend that someone should do this.

14. Eq. 5: do not use a differential for a finite difference (write with Δ instead).

15. Eq. 6, middle case: H has to be replaced by the fraction used in the other cases.

16. Eq. 8: It would be more easy to simply write h_t and h_b – full-word subscripts are not standard in math notation and a bit cumbersome.

17. Page 9, line 6: I don't think that you really mean *top of the atmosphere* here. Also, a few lines down, hs should become h_s.

18. Page 10: Do not write text in Eq. 9 in math mode, but add math mode for the eqations embedded in the following text.

19. Put "Eq." in front of the reference to an equation.

20. Page 11, l. 21, quote 'openair'.

21. Spelling of PM is inconsistent, sometimes PM2.5, sometimes $PM_{2.5}$, similar for PM1. For simplicity, I suggest not to use subscripts here.

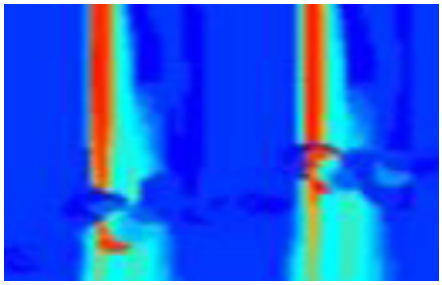
22. Page 13, l. 13, μ is missing.

23. Page 13, l. 16: "compared similarly" is not proper English. Line 20, not flights are "cloud-free" but the atmosphere probed. Line 20, "particle ammonium", probably "particulate ammonium".

24. Figures: Figures should be of uniform appearance and layout, and of professional quality. Some aspects that should be improved include

    - Do not frame the figures.
    - Axes, plot frames etc. should be in black, not in colour or light gray.
    - Do not use boldface in figures and use a sensible font size.

    - Move legend frames into corner of plot.
    - If there are subfigures, place a), b) etc. above or to the left of the subfigure, not within the plot.
    - Figure 3: The three subfigures show identical results, with the only difference that b) and c) zoom in on a part of the bins. This is not needed.
    - Figure 4: Again, zoomed versions are not needed.
    - Figure 5: The quality of the figures in insufficient; one can not see well the dots of the aircraft. I assume that those dots would be in the color corresponding to the airborne measurement even though this is not said explicitly. A part of the problem might be that dots are too big and overlap. A solution might be not to show many passes through the plume, but only a few characteristic ones with a better temporal resolution. I include here a zoomed-in detail of the plot to illustrate the quality problem.



    - Fig. 7: The background should not be white on light gray, but black on white. Also, make each plot square.
      The caption says that *plume-rise heights* are depicted, while the corresponding text (p. 24, l. 13) says that *plume heights* were calculated. As the physical stack height is not zero, this is not the same.
    - Fig. 9: The map scale is not readable in a) and c), while in b) and d) the

y-axis annotation is too tiny. Also, a geographical grid or coordinate axes are desirable for the map plots.

- Fig. 12a: Similar to to Fig. 5, the dots representing the aircraft measurements are not properly visible.

25. Tables: I hope that the table layout will be taken care of by the technical editor of ACP. Column headings should not be be broken within a word, and the use of italics and boldface has to be restricted to where it actually indicates something, not for the names of parameters etc.

26. Table 1: The full names of the metrics can go into the caption and the table itself would use only abbreviations.

27. Table 3: The caption should refer to the place where the abbreviations are defined.
The caption speaks about “concentration measurements” while the table reports ppb. Also, it is not stated whether mixing ratios are volume or mass mixing ratios.

28. Do not number the References section.

29. The following reference entries seem not to be mentioned in the paper:
EPA (no year) State-Level SO2 Data, Liggio et al. 2017, Vet et al. 2014. Note also that if there is no year, a text such as “no year” is usually substituted for it.

30. The following quotations in the text lack a matching entry in the References section:

    - Briggs (1985) quoted on p. 9, l. 22, is missing.
    - Coté et al. (1998), quoted p. 4., l. 6, is missing.
    - Im et al. (2015) quoted on p. 3, l. 2, lacks the a/b indicator.

    - JOSM (2011) is not labelled JOSM in the References.
    - Stroud (2008) quoted on p. 4, l. 13, should be Stroud et al. (2008).
    - Stroud (2016) quoted on p. 4, l. 11, is missing.

31. There are several instances of different spelling of authors’ names in the body of the manuscript and in the Reference section, e. g. Giebel vs. Gielbel, Hanna vs. Hann

32. The formatting of journal names is inconsistent.

33. The abbreviations used for journals are very short ones, not the standard, for example *Atm. Env.* instead of *Atmos. Environ.*, or even totally non-standard such as *J. of App. Met.*. The references to the ACP Special Issue on Oil Sands of which this manuscript is a part should be uniform.

34. EPA 2018 a and b lack a title. Also, if EPA 2018b is from 2015 as the URL suggests, why do you label it EPA 2018?