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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Understanding sources of organic aerosol during CalNex-2010 using the CMAQ-VBS" *by* M. C. Woody et al.

Anonymous Referee #2

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In this paper Woody et al., used the VBS approach in CMAQ to shed some light on OA sources during CalNex-2010. Their results highlighted the importance of meat cooking emissions over that region. However, while the model performance was improved compared to the standard CMAQ version (CMAQ-AE6) their model still seriously underpredicts OA which contradicts with numerous other VBS studies (i.e. Hodzic et al., 2010;Tsimpidi et al., 2014;Murphy and Pandis, 2009;Jathar et al., 2011;Shrivastava et al., 2011;Bergstrom et al., 2012;Fountoukis et al., 2015;Ahmadov et al., 2012). According to these studies, the use of the VBS approach greatly improved their model performance eliminating its underperformance regarding SOA. Therefore they should explain in a separate paragraph why their model failures to reproduce SOA mass (by a factor of five!) even with the use of the VBS approach. What is different compared

to other VBS studies? Is this attributed to some differences in the model set up or it is originating from local factors (specific for Pasadena)? Is there any other modeling study that uses the VBS approach in Pasadena that you can compare your results?

My second criticism is related to the presentation (mainly the structure and the writing) of the paper which I found it very poor. In their text they are making too big sentences, using too many numbers, and very occasionally they refer in too many information that is located in the supporting material (in total they have as much as 23 supporting figures) that makes it very hard for the reader to follow. So, even though I do acknowledge all the great work that the authors have done and all the significant and scientifically sound results that they provided through this manuscript, I strongly suggest them to go through the whole manuscript and make a thorough rewarding, delete all the unnecessary information, and use a more detailed structure to improve the presentation quality of their work.

To conclude, I do recommend this manuscript for publication but I advise the authors to make major revisions concerning the writing and presentation of their results. Through their work, especially through the sensitivity tests that they have conducted, they provide valuable information regarding the source apportionment of OA in Pasadena but also highlight the strengths and the weak points of the VBS theory. It is unfortunate to let the bad wording and complexity of text to shade the scientific findings of this work.

Bellow you can find some additional recommendations/corrections that I am suggesting for improving this manuscript.

Abstract

1. Please explain briefly the general characteristics of CMAQ-VBS against the CMAQ-AE6 simulation runs so as the reader can understand why there is an underestimation. In line 9 and line 12 the authors report this in parenthesis but it is insufficient. Please delete the parenthesis and explain a little bit more in a separate sentence.

2. Line 10. Please replace NMdnB with NMB throughout the whole manuscript

3. Line 23. Please explain what the term “intrinsic SOA” means before starting using it.

4. Line 20-24. This sentence is too big and too problematic. “based on species ratios”, which species and what rations? “SOA parameterization from the observation”, you mean SOA parameterization based on observations? In that case what kind of observations? The parenthesis used here are also confusing.

5. Line 27. “too low by about 7x”. In comparison to what?

6. Page 26747, line 3-8. Too big sentence. Please make shorter. Replace “compared to “ with “followed by”

7. Page 26747. How you estimated the 1.7 factor? This is based on SVOCs measurements?

Methodology

The structure of this section is inadequate. In several paragraphs the authors repeat same or similar information. The flow of the text would be greatly improved if the authors separate this section in subsections (i.e. 2.1 Model Description and Application, 2.2. Meteorology, 2.3 Emission Inventory, 2.4 Senstivity Simulations, 2.5 Measurements etc.). In addition this will help the reader to understand the main features of the model which unfortunately it is very difficult to be identified with the current format of this section.

8. Page 26750, line 8. Please report the actual value of the C* for the non-volatility bin used in the model. If it is set to 0 then you can mention that under typical atmospheric conditions at Pasadena this bin can represent all the compounds with C*$\leq$ 10-1 μg m-3.

9. Page 26750, line 10. Please rephrase. The sentence is too big and too confus-

ing. From my understanding the authors assumed that IVOCs are represented as a naphthalene-like surrogate specie and therefore they used the aerosol yield of ARO2 (which includes naphthalene).

10. Page 26752, line 8. What is the 10% here? (a) The 10% of the oxidation product is allowed to move to SOA and the rest remains as POA? Or (b) all the oxidation product is moved to SOA which is calculated to be approximately 10% of the reacted POA? If the (a) is correct then explain more the rationale behind this assumption. If (b) is correct please report this in your results and not here.

11. Page 26752, line 12-14. So a compound after 4 oxidation steps is still considered as POA? This is not correct. It should be compared against OOA and not HOA.

12. Page 26752, line 11-14. How much of the total OA is coming from the boundaries in your domain? You have to make a simulation without emissions to verify the assumption that is reported here.

13. Page 26752, the paragraph that begins in line 15. Here is an example of how confusing is this section. 4 paragraphs before this, the authors give some information of how SVOCs are treated in their model, then there is a paragraph with the model domain (which actually will fit better in the first paragraph of this section), then a paragraph with emissions used, then a paragraph with the meteorology, and then here they have an additional paragraph which again has information on emissions and how SVOCs are treated by their model. Please follow a more detailed structure and try not to repeat similar information.

14. Page 26752, line 26-28. Does the underlying chemical mechanism include species that are considered SVOCs or IVOCs (C*$\leq$ 106)? If yes please give a couple of examples. If it includes only VOCs then there is no double counting.

Results and Discussion

15. Page 26755, line 2. Delete “modeled OA”

16. Page 26755, line 15. Replace “or improve” with “resulting in degraded”

17. Page 26756, line 6-8. If CMAQ-POA includes OA from biomass burning emissions you have to compare the CMAQ-POA against the sum of AMS HOA and BBOA. Furthermore, you have to add LOA in the comparison. Is there any indication (or interpretation) on what is LOA (oxidized or not)? If it is considered aged material it has to be added to the comparison against CMAQ-SOA while if it is considered fresh it has to be compared against POA. Overall, you cannot compare all CMAQ-OA components against part of the observed OA except if you assume that you are missing a specific OA source that is attributed to a specific AMS OA type.

18. Page 26755, line 9. The authors switch randomly from OA to OC concentration or SOA to SOC through the whole text which I found it rather confusing and hard to follow. I strongly suggest the use of “OA” instead of “OC” and “SOA” instead of “SOC” throughout the text. Either way, the authors should report the factor used to convert modeled OA to OC (or measured OC to OA).

19. Page 26756, line 24-27. Can you make a small comment on how this scenario affected CMAQ performance regarding SOA?

20. Page 26758, line 22-25. This sentence is confusing. Please rephrase.

21. Page 26758, line 26. Please delete the whole sentence in the parenthesis

22. Page 26759, line 26. Add “that” after “suggest”

23. Page 26759, line 27. Add “therefore” after “2x and”

24. Page 26760, line 2. Add “which” after parenthesis

25. Page 26760, line 3. Add “that” after “assume”

26. Page 26760, line 4. Add “the” before “missing”

27. Page 26760, line 4. Has less impact on what?

28. Page 26760, line 5. Replace “or 25% excluding CIOA” with “(or 25% of POA excluding CIOA)”

29. Page 26761, line 16-19. Please rephrase. It is not clear how the numbers reported in this sentence suggest a factor of 2 error in the SOA precursor to CO emission ratio used by CMAQ

30. Page 26763, line 1. Add “that can” after “indicated”

31. Page 26763, line 13-20. Very confusing sentence. I can’t see any connection between the work of Jathar et al. (2014) and the sensitivities reported in this sentence. Therefore no conclusions can be made about the effect of Jathar et al. (2014) suggestions on CMAQ performance. Furthermore, the sensitivities reported here have not been presented earlier in the text. The authors should add a paragraph with all the sensitivities in the methodology section with their explanation and the rationale behind them. For instance, there is no point to use 7.5x POA emissions in this application. This has been chosen in Mexico City where the emissions where based on ambient measurements (which is not the case here).

32. Page 26766, line 7-8. Replace “the break down of POA was as follows:” with “POA comprised of”

33. Page 26766, line 24-25. Another example of bad writing. What kind of biogenics? More SOA at Pasadena than where? Or When? You can rewrite the sentence as: “The aging of biogenic SOA produced approximately 0.5 μg m-3 on average additional SOA at Pasadena throughout the day.”

34. Page 26767, line 11-12. Again, what kind of biogenic? Replace the sentence with “On the other hand, biogenic VOCs emitted in the Central Valley and surrounding mountains are thought to be the major source of biogenic SOA observed in the LA basin”

35. Page 26767, line 13-4. “underprediction of monoterpenes”: Do you mean under-

estimation of monoterpene emissions?

36. Page 26767, line 17. Replace “contribution for” with “contribution of”. Also, contribution to what? To predicted SOA concentrations?

37. Page 26768, line 4-5. Delete “has been presented (Hodzic and Jimenez, 2011; Hayes et al., 2015) and” and “here”

38. Page 26768, line 11. Delete “when”

39. Page 26768, line 15. Delete “and”

40. Page 26768, line 16-18. Delete the whole sentence. Unnecessary information for the purpose of this study.

41. Page 26768, line 19-23. There is no need for this to be in a separate paragraph. Also, you can reverse the order of these two sentences as follows: “In our implementation in CMAQ-VBS we use an emission rate of 0.069 g VOC* g-1 CO and a KOH=1.25 x 10-11 cm3 molec-1 cm-1. Hayes et al. (2015) found that using these optimal values, the SIMPLE parameterization...”

42. Page 26768, line 25. Replace “with the right diurnal cycle” with “following similar diurnal cycle” and place “(Fig. 9)” at the end of the sentence.

Conclusions

43. Page 26770, line 12. Add “from” after “50%” and “emissions” after “non-fossil”

44. Page 26770, line 15. Add “that” after “estimated” and add “the observed” after the “50% of”

45. Page 26770, line 16. Add “of SVOCs” after “66%”

46. Page 26770, line 20-27. I do not agree that is a matter of modelling needs and goals. During the last decade, the traditional treatment of OA has been proved to predict accurately the total OA in some cases (i.e., urban centers) but for the wrong rea-

sons (overpredicts POA and underpredicts SOA). Therefore, the traditional treatment should not be considered appropriate anymore. The only advantage of the traditional approach was its computational efficiency compared to VBS but this doesn’t seem to be an issue anymore for VBS approach since during the last 5 years it has been applied even in global models with great success (Pye and Seinfeld, 2010; Farina et al., 2010; Jathar et al., 2011; Jo et al., 2013; Tsimpidi et al., 2014). Please re-write the whole paragraph in order to highlight why the user has to switch to the CMAQ-VBS version by mentioning the great advantages of VBS (more accurate prediction of POA/SOA split without a significant computational cost)

Tables-Figures

47. Page 26781, line 10. Similar comment to the one above: the nonvolatile bin should represent all the compounds with C* $\leq$10-1 in Pasadena

48. Page 26786, Figure 2a. Did you convert AMS-OA to AMS-OC? If yes, which factor did you use? Furthermore, why there is no data for AMS during the period of 18/5-30/5 in figure 2a? According to Figure 2b it seems that there is available AMS data during this period.

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