Atmos. Chem. Phys. Discuss.,
https://doi.org/10.5194/acp-2019-986-RC1, 2019

Atmospheric Chemistry and Physics Discussions

Interactive comment on "Simulation of organic aerosol formation during the CalNex study: updated mobile emissions and simplified secondary organic aerosol parameterization for intermediate volatility organic compounds" *by* Quanyang Lu et al.

Anonymous Referee #1

Received and published: 18 December 2019

This paper discusses the hot-topic of IVOC emissions, making use of detailed emission inventory data and a new approach to SOA modelling. Overall the paper is well written, and the methods and asssociated data and assumptions well described.

Some issues which should be addressed are:

* The discussion of SOA yields and reactivity seems to be entirely focused on OH reactions. What about O3 and NO3 reactions?

* On page 4 it says that IVOC emissions are modelled based upon fuel type usage, but what about the emission control technology? I note that Lu et al (2018) commented that emissions show a consistency across sources for the same fuel type, but studies in other areas would seem to offer differing conclusions (cf. Platt et al. 2017 vs Dunmore et al, 2015 with respect to diesels.)

* The whole discussion is about IVOC. Cannot SVOC uncertainties also explain some of the results?

* The model evaluation is focused on just one site, Pasadena, except for some OA comparisons for six sites in Fig. 6. Although there may be good reasons to focus on Pasadena, the model results for other sites for pollutants such as CO or NOx should be briefly presented (maybe in SI). I don't think one can make very strong conclusions about the 'accuracy' or reasonableness of a SOA model based upon one's ability to reproduce observations at one site only, or of only SOA at six sites.

* The discussion of uncertainties from p10-12 was a bit confusing. Section 4, CMAQ simulation results, starts with predictions of IVOC at Pasadena. I would have preferred to see some model validation results first, before diving into the IVOC predictions. At this stage, we have no idea if the model works well for even the simple pollutants such as CO. Later (p12) we read about some NMOG comparisons, but those results are quite mixed (good for benzene, bad for toluene), so one can't be sure how accurate the NMOG inventory (or modelling) is. Page 11 manages to conclude that the uncertainty in IVOC is within a factor of 2 before these NMOG data are presented. Why, when some of the problems could reasonably be attributed to incorrect NMOG emissions? Also, p12 starts to attribute some problems to PBL height, but then the good agreement found for CO has to be explained.

Some small issues: ———————————

p2, L36, Abstract. With respect to SOA modelling, I am wary of phrases such as 'the most accurate photochemical model prediction'. It is always difficult to know if the improved performance is really due to a more accurate modelling system, or getting things "right for the wrong reasons". While I think the authors approach is generally as sound as one can do with SOA modelling, I would anyway rephrase to say something like "model predictions which are the most consistent with observations to date", or something similar.

p4, L102. What is meant by the quoted word enrichment? That word doesn't appear in the first two papers cited in that sentence (I didn't check the others).

p7, L194. What does 'remade' mean here?

p7, L201-202. It is stated that wind-blow dust should not impact comparison with data collected by AMS, but dust impacts nitrate formation (e.g. Hodzic et al., 2006) and indeed many gas-particle processes.

p9, L255-259. I think another important reason to not reduce VOC emissions is that this would impact the O3 chemistry in an unrealistic fashion. At least, unless you allow your IVOC to undergo gas-phase reactions, which I don't think is the case.

p11, L308. Language - emission inventories cannot be "correctly modelled".

p12. I don't think equations 2 and 3 are really needed, or should be moved to SI, since these are standard statistical metrics. If included (e.g. in Supplementary), then you have to explain 'Cov', 'Var', and N. You should in case explain though if you are taking statistics over hourly values. (The equations for FB and FE on page 15 could also be moved to SI.

p12, L363. OOA is not really "measured" by AMS; it is estimated through the somewhat subjective procedures of PMF.

p13, L389. Why 'However,'?

p14. With regard to these evaluations, I also wonder why biomass-burning, or COA are not addressed in more detail?

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p27, Table 2. This table gives the MW of the compounds. I am just curious - are the authors using these in their application of Raoult's law, or do they use the Donahue et al 2006 (Supplemental section) idea that one can use mass fraction rather than mole-fraction in the simulations?

p27, Table 2. Please be explicit that yields are mass-based.

p29, Table 4. The term traditional is starting to lose its meaning. Do you mean inventory or officially-reported POA?

p31, Figure 1. Give units.

Figs 2, 3, 6 and S1 had some formatting issues on my printer. Use a differnt graphics format if possible (.eps, .png?)

References

Dunmore et al., Diesel-related hydrocarbons can dominate gas phase reactive carbon in megacities, ACP, www.atmos-chem-phys.net/15/9983/2015/

Hodzic, A. et al, A model evaluation of coarse-mode nitrate heterogeneous formation on dust particles Atmos. Environ., 2006, 40, 4158-4171

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