Atmos. Chem. Phys. Discuss.,
doi:10.5194/acp-2017-193-RC1, 2017

Atmospheric Chemistry and Physics
Discussions

Interactive comment on "Semivolatile POA and parameterized total combustion SOA in CMAQv5.2: impacts on source strength and partitioning" *by* Benjamin N. Murphy et al.

Anonymous Referee #1

Received and published: 11 May 2017

In this work, Murphy et al. present the v5.2 of the Community Multiscale Air Quality (CMAQ) model, which takes into account the semivolatile phase partitioning and photochemical aging of POA emissions, and its evaluation over multiple seasons and locations. In addition, they have introduced into the model a new surrogate species that represents the potential SOA from combustion emissions (pcSOA) and explore its sensitivity to the emission scaling factor and the oxidation rate constant. Overall, the manuscript is very well written and the presentation is clear. However, I have a major concern regarding the implementation of pcSOA and the way that is presented. I recommend this study for publication after considering the following comments.

General comments:

1. The authors implemented pcSOA into CMAQv5.2 by using the SIMPLE parameterization for SOA formation in polluted urban regions Hodzic and Jimenez (2011). The optimal empirical parameters used for the formation of pcSOA (emission factors and oxidation reaction rate constants) are based on the observed proportionality of SOA concentrations and excess CO downwind of urban locations (i.e., Mexico City and Pasadena) under low biomass burning conditions. Therefore, pcVOC emissions includes all the anthropogenically emitted organic vapors and pcSOA expresses all the anthropogenic SOA. However, CMAQ already includes emissions of traditional anthropogenic VOCs and emissions of SVOCs (e.g., VSVPO3) and IVOCs (i.e., VIVPO1) in the gas phase, and therefore, the formation of SOA from anthropogenic VOCs, IVOCs, and SVOCs is currently double counted.

2. The first author of the manuscript have proposed a very effective nomenclature for atmospheric organic aerosols (Murphy et al., 2014). I would expect some consistency and I suggest to the authors to follow the naming convention of Murphy et al. (2014). In fact, the progress in the field of organic aerosols has come along with many complex and inconsistent abbreviates, therefore, adopting a standardized nomenclature will benefit the effective communication of the results to the scientific community. However, this is only a stylistic preference and it is up to the authors to adopt it.

Specific comments:

1. I find the introduction section very well written. Please consider including the following recent articles as well: Page 2 lines 24-25: (Shiraiwa et al., 2017); Page 3 line 10: (Ots et al., 2016; Jathar et al., 2017); Page 3 lines 19-20: (Ma et al., 2016); Page 4 line 1: (Tsimpidi et al., 2017)

2. Page 5 line 25: The Robinson et al. (2007) distribution includes emission factors up to the 106 μg m-3 volatility bin. However, CMAQv5.2 only have species with saturation concentration up to 104 μg m-3. Can you please include into the manuscript (maybe in Table 1?) the emission factors used for each of the primary organic material?

3. Page 6 lines 10-15: Does the oxidation of SVOC result in products with both higher and lower volatility than the precursor? I would suggest adding a reaction as an example and reporting the stoichiometric coefficients that you are using for each of the products.

4. Section 2.2: Do VOCs participate to only one oxidation step or are subject to multi-generational aging? Either way, I believe that SOA from anthropogenic VOCs is double counted due to the presence of pcSOA (see above in the first general comment). Hodzic and Jimenez (2011) do not include any traditional anthropogenic VOC specie (e.g., benzene) other than the lumped surrogate anthropogenic specie VOCA, which is analogous to the pcVOC used here.

5. Page 7 line 3: I am not sure that the name “pcVOC” is the more appropriate to use since this specie also includes unspeciated SVOC/IVOC emissions.

6. Page 7 line 25: The saturation concentration reported here (10-3 μg m-3) is not the same with the value reported in Table 2 (10-5 μg m-3).

7. Page 11 line 32: The sum of the fractions reported here is 99%.

8. Page 12 line 4: Please add the fractional biases of your nonvolatile POA simulation for comparison.

9. Page 19 line 31: Please consider deleting the “from anthropogenic and biogenic carbon sources”.

10. Figures 1, 2 and 3: Please add in the figures captions what the boxes and the whiskers represent

11. Figure 2: According to the figure caption, the observed values over Birmingham, Atlanta and Yorkville are organic carbon (in μgC m-3). Are the modelled values converted to OC as well? I would suggest converting everything (both observed and modelled values) to OA (in μg m-3) in order to be consistent with the values over Centreville and Look Rock, which are shown in the same figure, as well as with the title of the y axis.

12. Figure 3. Please add here (and discuss in the text) the model performance for POA and OOA over Centreville, Look Rock and Sacramento where there are also AMS measurements available.

13. Figure 5: I would recommend deleting the boxes and the whiskers behind each trend and keeping only the lines. This figure is too overloaded and it is very difficult for the reader to take any extra-information other than the trends of the lines.

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Interactive comment on Atmos. Chem. Phys. Discuss., doi:10.5194/acp-2017-193, 2017.