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Atmospheric Chemistry and Physics Discussions

# *Interactive comment on* "Simulating secondary organic aerosol in a regional air quality model using the statistical oxidation model – Part 2: Assessing the influence of vapor wall losses" *by* C. D. Cappa et al.

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The Statistical Oxidatiom Model (SOM) was applied to the South Coast Air Basin (SoCAB) and Eastern US as part of the UCD/CIT regional transport model. The focus was on examining how correcting for vapor wall losses might resolve model/measurement disagreement in terms of SOA magnitude, OC magnitude, and O:C ratios. The SOM model has many nice features, such as the ability to consider wall-loss and fragmentation/functionalization within the chamber fitting procedure as well as explicit predictions of the O:C ratio. The manuscript was well written and easy to follow. My comments are



aimed at clarifications.

Major comments:

1. Make sure that the terms used to characterize simulations as high vs low yield are precisely defined. In this work, high and low refer to the amount of wall loss in the chamber fitting. In Part 1 by Jathar et al., the high and low yield SOM parameterizations refer to low/high NOx regimes. This is potentially confusing to readers trying to follow the evolution of parameters through the literature.

2. Table 1: A correlation coefficient (Pearson's r, concordance correlation coefficient, etc) would be useful for model vs. IMPROVE/STN comparisons. Figure S4-S5 look like the correlation between model and obs might be low.

3. Simulations for 2010 (coinciding with CalNex) and 2013 (coinciding with SOAS/SEAC4RS) would be useful since concentrations have likely evolved significantly since 2005-2006.

4. Page 30091: How does SOM overcome the issue of dynamic range if it is based on the same chamber data as an Odum 2-product fit? While Figure S2 seems to show the Odum 2-product fits have some serious errors at lower delta(HC), are those lower delta(HC) constrained by the experimental data?

5. Page 30095: Is the high or low NOx regime more sensitive to wall-loss corrections? A column could be added to table S1 indicating the SOA yield (for a given set of conditions like total OA, etc.) relative to the uncorrected yield. What if instead of averaging the high/low NOx regime results, the authors only looked at high or low-NOx results? This would allow readers to infer their own SOA enhancements based on the relative dominance of the pathways. It appears that the low-NOx regime may be more sensitive to the wall-loss correction. In SoCAB, the high-NOx pathway is likely to be more relevant. Thus, figure 1 may overestimate the potential impact of wall-loss correction.

Minor comments:

6. Page 30085, line 10-11: Briefly recap how vapor pressure affects wall loss (decreasing vapor pressure leads to increasing losses?)

7. Page 30088, line 20: Should k_wall and alpha_wall also be mentioned as tunable?

8. Page 30090, line 6: In which direction is the correction conservative? High or low wall loss?

9. Page 30092, line 27: May want to mention that the CMAQ POA treatment by Simon and Bhave, although non-volatile, does account for aging of POA along a -1 van Krevlen slope due to OH reaction such that O:C evolves in that atmosphere (with a distinct diurnal profile).

10. Page 30094, line 1-4: While not always perfectly simulated, we do have some confidence in the ability of models to predict NO:HO2 branching. Models (at fine resolution, perhaps not at 36 km) capture spatial distributions in branching and GEOS-Chem captures seasonal trends in high vs. low-NOx isoprene oxidation products (Kim et al. 2015 ACP). I'm not sure if Carlton et al. 2010 is a good reference here.

11. Page 30096, line 1: This line reads that there is more absolute SOA over the ocean than land. Is that what was intended?

12. Page 30096, line 17-18, the authors may want to restrict the fSOA enhancements here to values from the Riverside or LA-Basin locations as higher ratios correspond to low absolute OA values.

13. Page 30099, was there an overall model bias in CO?

14. Page 30100: Keep in mind that NOx has changed significantly from 2005-2013 (e.g. Russell e tal. 2012 ACP) and that would affect the IEPOX-OA abundance. Changes in sulfate/acidity would also affect IEPOX-OA (e.g. Pye et al. 2013, Marais et al. 2015 ACPD).

15. Page 30102: The fraction fossil discussion that compares 2005 simulations to 2010



field data may need more caveats in its current form (ie highlighting potential changes in fossil fraction from 2005 to 2013). Could the authors not estimate the fraction fossil of SOC in the model given that the O:C ratio is known for the model species? That may eliminate some of the discrepancy in comparison.

16. Table S1 seems to indicate monoterpenes and sesquiterpenes have the same SOA yield. Why was that decision made?

17. What oxidants (OH, O3, NO3?) are considered for SOA purposes?

18. Figure 5: I'm surprised the base (SOM-no) simulation gets such high OA/CO ratios. In our CMAQ and CMAQ-VBS simulations (Woody et al. 20105 ACPD), we see slopes of 8 and 66 ug/m3/ppm compared to 108 in the observations for SOA/del(CO) vs. log(NOx/NOy).

19. Provide an estimate of the amount of computer processing time required for a SOM vs. base simulation.

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