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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Simulating the oxygen content of ambient organic aerosol with the 2D volatility basis set" *by* B. N. Murphy et al.

Anonymous Referee #1

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This is a nice, comprehensive study looking at simulating oxygen addition with aging using a Lagrangian model and comparing with measurements from FAME-08. The presentation is clear and I have no major critiques of the methods or results. My suggestions below are mainly to clarify the presentation and context of the results.

1. The FAME-08 data are not a stringent test of model performance of aging given the consistency of observed of O:C and OA mass concentrations. It's not clear that the model would capture the variability in these parameters, as they might exist in a region influenced by a variation of air mass ages. Now clearly there are not many alternate datasets available at this time, and I am not suggesting that additional cases should be added to this study. However I think this aspect of a weak test case with limited dynamic range should be (strongly) emphasized in the discussion.

2. Given the complexities of simulating all OA formation processes, including those (very reasonably) not included here, but discussed by the authors in the text, there is at times an inappropriate degree of confidence in the current results. This should be toned down. For example, fragmentation processes (ignored here) could lead to reductions in OA mass and likely increases in O:C. This could compensate for the high OA simulated when both aSOA and bSOA are aged. Overall, I think it should be emphasized that though you have pursued a nice series of sensitivity tests here, your system is underconstrained and you cannot definitively conclude regarding model performance. Text should be modified throughout Sections 4 and 5, specifically

a. Page 8554, lines 23-25

b. page 8574, lines 21-24

c. page 8575 line28 through page 8576 line 6.

3. On a related point, it seems completely arbitrary to age aSOA but not bSOA. The text suggests that this approach is considered in the best case solely because it is the "best fit" to the measurements. If not, please provide some justification. If so, please refer to above point.

4. It's unclear why so many of the plots are represented as diurnal means given the very, very small degree of variability in the time dimension. While it is interesting to see the modeled difference in O:C throughout the day in Figure 3, others (such as Figure 4, 6 and even 2) are not particularly informative as shown.

5. Page 8562, line: 28-29: Can you provide some chemical justification for the addition of one or two oxygen atoms per reaction with OH in the text?

6. Page 8563, lines 27-28: Can you tell us in the results what the average increase in mass in your model simulations is to compare with the prior assumptions by Lane et al. and Grieshop et al. ?

7. Page 8568, lines 7-8: Are MEGAN emissions calculated online in your model or

taken from an offline calculation (if so, please specify)

8. Page 8568, lines 10-13: You need a reference for the sea spray source function parameterization (O'Dowd et al. is the partitioning of sea spray reference only).

9. Page 8569, lines 1-2: How much chemical uncertainty is associated with clustering these back trajectories? I assume little given the consistency of the aged air masses, but it would be worth testing this for a day (run the chemical model for all the back trajectories and look at the variability) and stating so in the text.

10. Page 8569, lines 4-5: Please specify in the text whether the initial conditions from PMCAMx are matched for the same date and time of the back trajectories or a climatological mean.

11. Page 8569, lines 20-21: Please provide more information on the simulated bcOA. Is this a constant advected in from all directions? What are the likely sources?

12. The supplementary materials are brief and should be re-integrated into the main text. Figure S3 is unnecessary given the discussion in the text. You could perhaps add a mean map of emissions for the region to underly Figure S2.

Interactive comment on Atmos. Chem. Phys. Discuss., 11, 8553, 2011.