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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Simulation of Atmospheric Organic Aerosol using its Volatility-Oxygen Content Distribution during the PEGASOS 2012 campaign" *by* Eleni Karnezi et al.

Anonymous Referee #2

Received and published: 5 March 2018

Summary/recommendation: This paper seeks to model total OA concentrations and O:C ratios from ground and airborne measurements from the PEGASOS field campaign. A number of chemical aging schemes were used, and although several schemes performed well, no one chemical aging scheme yielded superior model-measurement fits. This is a well-conducted study and I recommend that this paper be in published in ACP but with revisions, as discussed below.

General Comments:

Pg 3 lines 65-67: is this paper also using all those classifications of OA? Not clear from the "Lagrangian CTM description section". How do you distinguish SOA-sv and SOA-iv

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from and/or between aSOA-v and bSOA? In general, this work assumes a knowledge of the Murphy et al. 2011 and 2012 papers and model that the modelling work was built upon. As a reviewer not familiar with the model used in this work, it was difficult to follow some of the more complicated nuances of how the model treats different OA types. I suggest that more details about the model be added to assist the reader.

Sec 2.2.2: Need to give clear justification as to why there are two aging schemes of bSOA, and not any other type of SOA. These details need to be included.

Pg 6, simple scheme description: were any sensitivity studies done on the rate constants used for reactions with OH? A comment should be included about this assumption.

Pg 10, Lines 299-300: There could be a brief discussion here of the potential problems of basing best-fit model conclusions on just one flight.

Sec 3.4 How valid is it to tune fragmentation to the measurements with just 7 cases?

–It's confusing in general how many cases were used and how the averaging was done with the model and measurements, especially between ground based and zeppelin measurements, since many of these didn't match in time/date. This should made clear throughout the manuscript.

–It would be good to include a brief discussion of uncertainty related to model emission inventories, if any details of this are known (e.g. other model-measurement validation studies).

–Ultimately, aging schemes are tuned to fit the measurements and 7 different aging schemes are found to well-reproduce the measurements. However, this paper did not provide any or enough discussion about measurement uncertainty, number of measurements, or the other uncertainties I brought up above (emissions, rate constants) to allow the reader to firmly conclude anything about the validity or transferability of these tuned best-fit schemes.

–I feel that it would be of interest to the community to provide a brief discussion about the pros/cons of the different aging parameterizations used in this study. E.g. the simple functionalization scheme could be implemented into a more computationally intense model (e.g. a global CTM) but potential could have biases from leaving out Y; the detailed functionalization scheme provides X extra information but is likely unrealistic in Z, and so forth.

Figures/Tables: Figure 5: is the average OA from the ground measurements or does it include the zeppelin measurements? Caption and text should state this clearly. Figure S3: it would be helpful to each SOA type (ASOA-v, bSOA, etc) and the case types redefined either in the caption or in a brief section before the figures redefining both the SOA types and the case types. The case types are defined nicely in Figure S5 but that doesn't help out Figure S3.

Technical comments: Line 233: what is Figure C.4? Line 272: no comma after "predictions" Line 311: no comma after "scheme" Line 400: finish parenthesis

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