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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Simulating the detailed chemical composition of secondary organic aerosol formed on a regional scale during the TORCH 2003 campaign in the southern UK" *by* D. Johnson et al.

Anonymous Referee #1

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General comments:

The manuscript presents the chemical speciation of SOA compounds both from anthropogenic and biogenic sources by using a box model based on the chemical mechanism MCM3.1. The work presented is original and I recommend to be published in Atmospheric Chemistry and Physics. However, the manuscript requires some major improvements prior its publication.

Specific comments:

1) Although the model has been described in detail in the companion paper by Johnson et al. (2005), there are some important assumptions that are being made and need to be emphasized in the current paper. The assumption that POA emissions are relative to NOx emissions is valid only for the location that the measurements are made, and not to all countries that the air-trajectory passes through. The same applies for the POA/BC ratio. The "ubiquitous" concentration of OA, the increase of the partitioning coefficient by a factor of 500 (uniform to all species) are also factors that require more explanation.

2) Especially concerning the uniform increment of all partitioning coefficients by a factor of 500, an explanation is needed whether or not this number comes from a scientific argument or just to fit the measured concentrations. Since there is an indication on the accretion reactions that might take place (page 7885 line 29 to page 7886 line 2), why not using different factors for different compound groups? Since the detailed chemical composition of SOA is the main interest of this work, as mentioned in the title, applying different incremental factor to the partitioning coefficients of multi-aldehydic compounds will change both the gas-phase chemistry and the chemical composition of SOA, altering (a lot?) the results. More discussion is needed on this respect, if not a couple of sensitivity model runs with different incremental factors of the partitioning coefficient for different types of semi-volatile compounds.

3) Additionally to table 1, it would be very interesting to present a table with the relative contribution of each functional group (e.g. aldehyde, ketone, acid, alcohol, nitrate, peroxy) to the total SOA mass.

4) When discussing the results, it would be more convenient to the reader to declare the letters of each one of the case studies, like in the footnote of table 1, instead of (or additionally to) the date (e.g. page 7887 line 26, page 7888 lines 6 and 14).

5) Table 4, line 6 - a/(a+b): Since the chemistry is not linear, you cannot make this

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% contribution calculation. Instead, you can make a model run with increased both the anthropogenic and biogenic VOC emissions by 10% and use this number as the denominator.

6) Figure 2: Since you assume that accretion reactions occur, I would expect that isoprene also contributes to the SOA mass. A increasing number of papers appear in the literature concerning the isoprene contribution to SOA mass, which should be taken into account in your calculations. This assumption looks even more strange when reading that benzene is also included in the precursor VOC of SOA, when literature in most (but not all) cases says the opposite.

7) The effort made to attribute each one of the products to specific parent VOC, although interesting, can confuse the reader. It is difficult to get clear conclusions when using at the same model 124 anthropogenic compounds and only 3 biogenic, especially when knowing that compounds like limonene are also abundant and more SOA efficient. Sesquiterpenes, even when not being so abundant, have also high SOA yields. A small discussion about the biogenic parent VOC lumping whould be useful.

Interactive comment on Atmos. Chem. Phys. Discuss., 5, 7875, 2005.