

## ***Interactive comment on* “Simulating regional scale secondary organic aerosol formation during the TORCH 2003 campaign in the southern UK” by D. Johnson et al.**

**Anonymous Referee #3**

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### **General comments**

This paper on the constitution of ambient organic aerosol masses during the TORCH 2003 campaign using the highly detailed MCM 3.1 for gas-phase simulations is highly interesting. Not only because of the general approach of using back trajectories and simulating the general contribution of e.g. primary organic matter and secondary organic aerosol matter but also by applying the immense details of the MCM chemistry and its impact on the aerosol formation process this study increases the knowledge of

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organic aerosol precursors at least for the UK during the campaign and I would like to congratulate the authors for their goals and results.

## Specific comments

There are some aspects worth spending more discussion about and a few questions arose during reading. First, why do you apply always an ubiquitous background concentration of  $0.7 \mu\text{g m}^{-3}$  for the simulations? You state correctly that in fine particles the organic mass contribution is found between 10 and 90A second question came up when reading about this 'scaling factor' of 500, with whom the calculated partitioning coefficients had to be multiplied in order to gain the observed organic aerosol mass loadings. One explanation might be the difficulty in estimating the true saturation vapour pressure of the different participating compounds. E.g. for pinic acid the saturation vapour pressure with a boiling point of 612 K [Jenkin et al., 2004] at is calculated to be  $6.15 \times 10^{-2}$  Pa, whereas the direct measurement of Bilde and Pandis [Bilde and Pandis, 2001] yields  $4.36 \times 10^{-5}$  Pa. The discrepancy is about 1400, even larger than the factor of 500 used in here. And pinic acid is usually one of the best known compounds among the huge number simulated in the accompanying paper [Johnson et al., 2005b]. But what I was confused with was that this number had to be increased from earlier smog chamber studies [Jenkin et al., 2004], which claimed it to be between 5 and 100 as stated well in the present paper. If there would be an overestimation in the vapour pressure it should be similar in both cases. But of course temperature might play a role in here.

This leads to the effect of using two surrogates for all monoterpenes and higher terpenes. Of course even a more detailed investigation would lead to an 'explosion' in the number of reactions to be treated, which can't be done even in a box model for this study. However, assuming even more terpenes, aromatics etc would split up the

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number of compounds even further, leading to smaller individual concentrations and smaller partitioning of these. Consequently, this approach should overestimate the mass production slightly instead of underestimating it.

What about heterogeneous reactions [Jang et al., 2002; Barsanti and Pankow, 2004; Kalberer et al., 2004]? Within the assumed very long lifetime of tropospheric aerosols in here these should occur and matter, when simulating several days but not in the smog chamber studies.

Finally, just as a curious question, what do the authors think about the influence of larger compounds, more reactive like sesquiterpenes, which are usually extremely hard to detect and below of most instrumentation detection limits. However, due to their more than 100 times faster reactivity with respect to ozone they will impact strongly on the ozone concentrations during the day and from my latest knowledge their emissions do not necessarily correlate with the one of monoterpenes. I would be interested in the impact of these on the presented results and if they could explain some of the scaling performed.

## References

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