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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Global modelling of secondary organic aerosol in the troposphere: A sensitivity analysis" *by* K.Tsigaridis and M. Kanakidou

Anonymous Referee #2

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The paper evaluates the sensitivity of the Secondary Organic Aerosol (SOA) predictions of a global 3-D Chemical Transport Model to a number of model parameters (thermodynamic parameters of the SOA species, reactivity of the first generation products, etc). The results of the analysis explain the relatively wide range of SOA levels predicted by previous modeling efforts and suggest areas where future work can reduce the uncertainty.

Major comments

1. *Comparison with laboratory results*. A model including both first and second generation products is presented here using parameters derived from smog chamber experiments. However, it is not clear how well the model reproduces these smog chamber

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results. A section comparing the model predictions with the smog chamber results should be added.

The importance of the secondary oxidation reactions is not clear in the paper. It appears in Table 6 that it has a relatively small effect in the model results. Some additional discussion is needed.

2. *Choice of scenarios for simulations*. It is not clear what scenarios S3 and S4 represent. According to their description they include partitioning of SOA on sulfuric and ammonium aerosol. Do the authors assume that SOA forms a solution with the sulfates and ammonium? Do these scenarios describe dissolution of the SOA in the aqueous aerosol phase? No information is provided about the activity coefficients used for the different solutes in this case. The authors should describe clearly the physical basis for these scenarios and the corresponding modeling. If these scenarios do not have such a basis, they may want to consider removing them from the paper

The no-evaporation scenarios (S2 and S4) are also a little confusing. Do the authors assume that the SOA species have zero vapor pressure at all temperatures and therefore their transport to the aerosol phase is irreversible? The SOA partitioning algorithm for these scenarios should be explained.

The sensitivity to the primary organic aerosol emission should be tested. The authors realize that their inventory probably underestimates these emissions, but they do not attempt to double the corresponding emissions.

The importance of the treatment of the removal processes should be discussed a little more. The model describes the hydrophobic to hydrophilic transition for these species, but the importance of this process for the SOA burden is not investigated.

3. *Presentation of the sensitivity analysis results*. The presentation of the results should be improved. The reader does not get a good sense of the importance of the different parameters because the discussion focuses on the details of the spatial

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SOA distribution and not on the integral measures (e.g., chemical production, burden) of Table 6. The discussion is also a little misleading sometimes. For example, it is not clear that the activity coefficient does not make much of a difference.

Several figures can be deleted to reduce the length of the paper. They include most of the figures from the sensitivity analysis (Figures 6, 7, 8, 9, 10, and probably Figure 3). Table 6 and the discussion in the text are sufficient for the presentation of the results.

4. *Synthesis*. A clear section synthesizing the results and making recommendations for future research would be useful. The results suggest that while some parameters and processes are important some others are secondary. Both of these types of processes should be discussed quantitatively.

The authors could use the comparison with the observations here to say something more about the different scenarios despite the uncertainty of the primary OC emissions. Are the high and low SOA estimates reasonable when one considers the measured concentrations?

Minor comments

5. *Numerics*. The numerical scheme for the solution of the system of equations is not described well at the top of page 7. It appears that the authors reduce the system to one algebraic equation with one unknown (Mo) and then use an iterative procedure. The numerical scheme should be clarified and its computational requirements should be discussed.

6. *BC data*. I would not describe the performance of the model with BC as good (page 12). It appears that roughly half of the points are more than a factor of two or three away from the measured values. May be providing some statistics of the performance instead of a qualitative statement would help.

Interactive comment on Atmos. Chem. Phys. Discuss., 3, 2879, 2003.

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