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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Parameterising secondary organic aerosol from $\vec{\alpha}$-pinene using a detailed oxidation and aerosol formation model" *by* K. Ceulemans et al.

Anonymous Referee #1

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This paper develops a parameterized model for alpha-pinene oxidation under different atmospherically relevant conditions interestingly using an explicit alpha-pinene oxidation chemistry box model.

The advantages of this approach are obvious: 1. A box model, unlike smog chamber experiments, provides flexibility for considering different conditions for SOA formation. Hence, more generalized parameterization is possible 2. The total yields include the process of ageing, since the model is run for numerous days (24 days), till the concentration of SOA reaches near equilibrium.

Initial comments

I liked the idea that that many different features of SOA formation such as liquid water content and low NOx,etc. are addressed in this study. Initial concerns are that comparisons with just SOA max form different chamber studies are presented as opposed to showing how their simulations fit the entire SOA time concentration profile as SOA is being generated in the different chamber studies. It would also help the reader if similar simulations of SOA profiles from different chamber studies with the full-blown BOREM model could also be shown, since it what the parameterized model in this study is supposed to be simulating. In addition the paper could be dramatically strengthened if comparisons with the VBS modeling approach could be shown for, again the same chamber data.

Further comments

1. The biggest concern is the issue of prompt production of SOA products if such a parameterized model is implemented in a global model. For example, much of the higher yields obtained in the low-NOx scenario is due to several days of ageing. However, implementation of a parameterized model developed here (that implicitly assumes yield from ageing) will lead to prompt SOA production for each timestep, leading to overestimation of SOA at shorter time-scales. In that context, the VBS method with ageing allows representation of SOA formation at different time-scales and might turn out to be more accurate temporally. One interesting approach to be considered to address this concern is to introduce SOA parameterization based on ageing. The implementation of such a technique in a global model can be implemented by tracking the age of the reacted alpha-pinene mass.

2. 10-product model is a misleading term. The box-model essentially is used to get parameters for a 2-product model, albeit for 5 different starting conditions. This is equivalent to performing 5 sets of smog chamber experiments and fitting a 2-product model for each set. I would suggest not using the term 10-product model as it can be misleading to the readers.

3. Have the authors considered a condensed kinetic lumped product technique instead of the 2-product model approach? This again can help the accurate kinetic representation of the process of ageing, currently a big uncertainty for global models

4. This approach might be harder for aromatics and isoprene, where the explicit chemistry is not fully developed, particularly particle-phase reactions. Also, the effects of types of seed and lower concentrations of seed is harder to quantify in a parameterized model.

Interactive comment on Atmos. Chem. Phys. Discuss., 11, 23421, 2011.