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Discussions

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Interactive comment on "Model-measurement comparison of functional group abundance in α-pinene and 1,3,5-trimethylbenzene secondary organic aerosol formation" *by* G. Ruggeri et al.

Anonymous Referee #3

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This manuscript introduces a modelling method than can be used for simulating secondary organic aerosol (SOA) formation and for studying especially functional group (FG) contributions in SOA. This kind of modelling approaches are necessary steps towards understanding SOA formation. The modelling framework is reasonable, manuscript is well written and the topic well within the scope of ACP. Therefore I recommend publication of the manuscript in ACP after minor revision.

Specific comments:

1) There are number of assumptions/estimations/simplification included in the model and the effect of these on the model results and for model-measurement comparison has not been discussed. Authors state that the relative abundances of functional

groups are robust with respect to many of the assumptions (P. 4, L. 23-24). However, I feel this statement needs to be justified. I recommend adding a short discussion/statement on the effect of the following:

a) Fixing radiation intensities in the model one constant value (P. 4, L. 6) Does this correspond to conditions in the experiments? If not, are the simulation results sensitive to this?

b) A seed is used for initializing the gas-particle partitioning (P. 4, L. 14-15). According to the appendix A the initial seed composition is calculated based on equilibrium gas-particle partitioning theory. Can this initial composition affect the model results at short simulation times? Also, I recommend adding here in the main text a sentence about how the initial seed composition was assigned.

c) The vapor wall losses where neglegted (P. 4, L. 20). Could this affect the simulations as the wall losses are likely volatility dependent and therefore may affect different FG differently?

P. 5, L. 24: 'FTIR analysis has been found to measure around 80 % of the organic mass...' How does the remaining 20 % affect the model-measurement comparison? Could the differences between modelled and measured FG relative contributions be explained in some cases by the missing 20 % of organic mass in measurements?

P. 8, L. 1-2: In addition to missing particle phase aggregation reactions, also highly oxidized high-molecular mass gas phase products might be missing from the model (Ehn et al. 2014, Nature 506, 476-479. Could such highly-oxidized organics explain the discrepancy between the model and measurement?

P. 13, L. 19-21: Here it would be good if the authors could summarize also that in which conditions their modelling tool may be applicable and what kind of improvements would be most important ones.

Authors mention that for APIN-hNOx and APIN-nNOx cases the model underestimates

the SOA mass by an order of magnitude. I was missing this information for the cases APIN-lNOx and TMB-lNOx.

Technical comments:

P. 7, L. 30-31: 'The sum of the oxidized fraction in the simulation. . .' This sentence is unclear, please revise.

P. 11, L. 14-26: Why are the model results here compared to Sato et al. measurements although the model simulations were designed to simulate the Sax et al. measurements?

Figure 2: Please clarify what 'relative mole fraction compared to the first sample' means. This can be interpreted at least as a ratio between molar fractions of compound i at time t and time t=0s or as moles of compound i at time t divided by moles of compound i at time 0 s.

Figure 2: Please clarify if the naCO includes both ketone and aldehyde for the model or if naCO includes only aldehyde for the model as ketone is presented also separately. At the moment it's not clear in measured naCO should be compared to modelled naCO or the sum of modelled naCO and ketone.

Figure 2: Consider plotting a vertical line at y = 1.0. That would make it easier to read the figure in case of those compounds that show only small changes.