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Interactive comment on "Development of aroCACM/MPMPO 1.0: a model to simulate secondary organic aerosol from aromatic precursors in regional models" *by* M. L. Dawson et al.

Anonymous Referee #1

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General comments:

Xu et al. (2015) have further developed the module called aroCACM/MPMPO 1.0 in order to simulate secondary organic aerosol mass (SOA) from aromatic precursors. This study is a follow-up investigation on modifications performed on the module with a special focus on different environmental NO_x conditions and its implementation into the regional air quality model CACM.

The authors focussed on a smaller subset of aromatic species and related gas-phase chemical reactions because of the limited amount of simulation time for any regional

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model. While being constrained by simulation capacities earlier studies (Seinfeld and Pandis, 2006; Ng et al., 2007; Xu et al., 2015; Im et al., 2014) have expressed the need to resolve the effect of NO_x on the details of volatile organic compound (VOC) oxidation and subsequent SOA formation. This was considered by concentrationg on two exemplary aromatic spieces only, i.e. toluene and m-xylene as representatives for the other aromatics and their corresponding lumped chemistry. The precursor VOCs and their oxidation products were splitted into low and high-SOA-yield species according to the MPMPO scheme (see Xu et al., 2015). Several improvements recommended by Ashworth et al. (2015) were made. Those include increasing the contribution of hydroperoxy and organic peroxy radical reaction rates by increasing the related reaction rate constants. The new implementation of SIMPOL.1 for estimating compounds saturation vapour pressures was well done and important. And the daily variation of SOA types contributions is quite nice.

Detailed comments and questions

Overall, the study by Xu et al. is easy to read and provides some new findings, but is written in a sometimes rapid style and some aspects questions should be clarified in a better way before final acceptation. Those are:

p. 2: Aromatic species were named to react with OH, NO_3 and chlorine radicals only. This is true for all the explicitly named and most of the aromatic species except styrene, which may react with ozone too (Atkinson et al., 2006). Although being a minor contribution to the total petrol vapour concentration usually observed the SOA yield by styrene + ozone will be substantially larger as ozone reactions yield substantially less volatile species (Hallquist et al., 2009).

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p.5 (general): I would recommend providing a supporting only information document as several essential details of former studies are not directly available. This would help the reader understanding the study details much easier than to read in all the precessing articles. It includes a table of all the SOA groups and corresponding marker species (before and) after the modifications. An overview plot within the study may ease the understanding of the change when splitting B4. Parts of that Table can be found in Tables 1 and 2 as well as in Figure 1. A second aspect worth mentioning covers the initial conditions of the experiments displayed in Figs. 2, 3 and 5-8. Was an initial amount of seed aerosol introduced for partitioning calculations and if so which amount? Or was the system treated clean and the SOA had to form out of the gas-phase via new particle formation? This may cause a changing saturation vapour pressure because of Kelvin effects. The consequence would be time delays in experimental observations and challenges for simulation as partitioning requires an at least infinitesimal amount of pre-existing SOA mass. Was there a spin-up time assumed? Did the authors exclude certain data that were out of a certain range? In which concentration range of organic aerosol (OA) the authors would classify the approach to work properly and in which not?

p. 8: I would favour some "rapid writing style" improvements such as for "Ashworth et al. (2015) reported several updates to CACM (what they termed CACM0.0)...The rate constants for the reaction of organic peroxy radicals (RO_2) with hydroperoxy radicals (HO_2) or other RO_2 species were increased to be in agreement with Table A2 in Ashworth et al. (2015).". Both rate constants were increased by which factor etc? Was the change substantial i.e. affecting any of the results displayed later on? Note Ashworth et al. (2015) did a forest study while this study deals with urban areas and does not include other biogenic VOCs than isoprene.

p.9 (general): The redistribution of class B4 to subspecies and the related results left me somewhat puzzled when looking at Figure 3. While the saturation vapour pressure estimation had a notable (+1 $\mu g/m^3$) effect the daily pattern remained unchainged.

Both rush-hours are visible at different intensity, which agrees with the different mixing layer height and dilution. This daily pattern is not obtained for the simulation of the redistributed B4 SOA class that basically shows an inverse daily structure of a mixing layer height and substantially lower formation yields. In typically elevated urban conditions I would expect to obtain similar results for a lumped compound class and for the individual compounds if using the Pankow (199a, 1994b) approach, since there is no condensation but partitioning taking place at any concentration level. My two only explanations for that would be (i) one of both approaches used a completely different saturation vapour pressure or (ii) the preexisting organic aerosol mass is subestimated with a negative feedback on the formation rate. Thus, I don't know which of both simulations to trust as no observations are displayed for quality check. For a better understanding I would recommend a replacement of the class numbers like A1 by a structure based name in Fig. 3, as the abbreviations have not been explained all in the text and one could easier identify the respondible group for the deviations.

p.11: It makes me struggle somewhat that the authors used nicely the SIMPOL.1 approach (Pankow and Asher, 2008) for a better saturation vapour pressure estimation but adjust it afterwards to match the former results by Xu et al. (2015) at a temperature of 25 degrees C. Did the authors not trust the SIMPOL.1 estimates? Was the approach used to get the relative list (volatile, semi-volatile, non-volatile compounds) in the correct shape but control the absolute values? Please explain.

General: A key feature for every experiment and simulation approach - not this one exclusively - should be a statement in which range a certain approach provides reasonable estimates (valid range). This would force future users to carefully consider not a "black box" for application and take it into account for interpretation of results. Could the authors provide such to make a future application as appropriate as possible and potentially name issues with a need for further improvement? That could serve as new standard.

Finally one question about other SOA precursor and compounds was left: So far larger

biogenic VOCs such as monoterpenes are not included probably because of simulation capacities and lack of informations. Those are much less volatile and would allow a higher preexisting mass present for partitioning of aromatic compounds. Did the authors made tests on the sensitivity of the simulations to preexisting particle mass?

p. 24 and 26 (Fig. 6 and 8): I guess the apparent notable presence of furanones and tiny amounts of epoxides in Fig. 6 can be explained by the primary focus on AROH emissions. Correct?

p. 26 (Fig. 8): The daily structure of PAN-like species and epoxides is very interesting and matches with expectations. Could you provide a standard deviation (variation) of your mean model domain pattern for the 5 classes?

If those issues are clarified the study deserves publication in Geoscientific Model Development.

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