Interactive comment on “Multi-generational oxidation model to simulate secondary organic aerosol in a 3-D air quality model” by S. H. Jathar et al.

Anonymous Referee #1

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The paper of Jathar et al. presents a new approach of SOA prediction. The statistical oxidation model (SOM) was incorporated into SAPCR-11 in a regional air quality model (UCD/CIT) in order to simulate the SOA gas/phase partitioning and the oxidation of the multi-generation SOA by OH radicals, including both functionalization and fragmentation. The significance of such predictions is high, as SOA often constitutes a large fraction of the organic aerosol (OA). The topic is relevant to the GMD. The manuscript is well-written and the overall quality of this work is good. I recommend publishing of this paper after the following major additions:

The outputs of this model (SOA concentrations and O:C ratios) are of major importance, but how well they represent the ambient atmosphere? There is no comparison with measured data. The authors should select domains and periods where ambient data from AMS are available. A comparison between the modeled SOA and total OOA extracted by PMF (i.e. sum of SV-OOA and LV-OOA species) is necessary for the evaluation of this model. The idea of handling together fragmentation and functionalization processes is important; however, it has to be evaluated against real ambient data. Though the predicted SOA concentrations are in the range between 0.3 and 2 \( \mu \text{g m}^{-3} \), which is a logical range, the spatial concentration distribution could be very different compared to ambient measurements. Concerning the O:C ratio the authors use a short and very general statement (page 1877, lines 4-6) to justify their results, which is very weak. O:C also has to be compared with measured values. Even if the average O:C range is within what is globally seen it does not mean that spatially the model reproduces the correct values. This has to be proved.

The authors should evaluate this model. In my opinion, without comparisons to ambient measurements and evaluation of the predictions, this paper is very weak.