

Interactive comment on “Impacts of water partitioning and polarity of organic compounds on secondary organic aerosol over Eastern China” by Jingyi Li et al.

Anonymous Referee #1

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The authors present model results using the WRF/CMAQ for SOA formation in China. The model is updated for the partitioning of water vapor to the organic aerosol and the non-ideality of the organic phase. A comparison of the model to observations is performed for multiple sites. SOA enhancement during the summer and winter is discussed for the different China domains. The effect of aerosol liquid water on SOA formation and aerosol optical depth are presented. Correlation of the calculated OA hygroscopicity based on the k-Köhler theory to the O:C ratio is performed to show seasonal and multicity variations. Although the publication could provide valuable insights into the factors that govern SOA formation in China it currently lacks a detailed discussion and validation of the presented results. Therefore, the publication requires major

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revisions suggested below.

Major Comments

The manuscript is hard to read. Discussion and Results are not well separated in the manuscript. Many phrases are not clear and require more elaboration and better use of English. The table and most figures are poorly made and the science is hard to follow. Examples are given below.

A major drawback in this work is that the model is not capturing the SOA formation during the winter that has been shown to be the dominant organic aerosol source in multiple publications for different domains of China. The authors only in a sentence discuss that the conversion of the POA to SOA may be the reason for these discrepancies but they have no observations to back this up.

There is no discussion on the influence of nitrate on aerosol liquid water. What fraction of the ALW is related to nitrate and what to organics? How could the ALW related to nitrate influence the partitioning of organics?

A comparison of the model to observations should be performed and presented in the main text for both seasons in more detail. The effect of the improvements performed for the SAPRC-11 model is not discussed. The processes added e.g., the heterogeneous formation of nitrate and sulfate on the particle surface, SOA from isoprene, and dicarbonyls surface-controlled reactive uptake are not discussed. What is the effect of these added processes to the overall performance of the model? Each addition and the effect should be discussed in detail in order to support the importance of including them.

MEGAN has been shown to overestimate the isoprene emissions. Would this have a major effect on SOA formation in this work?

Table 1: There is no discussion of the table in the main text. Abbreviations are not included in the caption. What is MB, GE, Num? Discussion on more statistically rel-

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evant values would be beneficial, e.g. what is the R2 of the comparisons? What are the presented values? Medians? Means? What is the domain of the model and how much do the values fluctuate around the domain? What are the uncertainties of the measurements and the model? A figure of the comparison of temperature and relative humidity of obs. vs model with the associated errors and linear regression analysis with the statistics would be informative.

Figure 1: The current Figure has no information regarding the season the measurements are performed. A comparison of both seasons should be made and a figure like Fig1(a) should be made for each season. The timeseries should include the same site for the two seasons. Why is the base case exactly the same as the S3 in Figure 1(b)? Add errors to the measurements.

Figure 2: Why do you use in (a) the base case and not the S3 case? I would consider promoting the updated S3 on the left and the changes on the middle and right panels.

Figure 3: I don't see the point in presenting the ratio of LWCorg to SOA. If both are expected to increase during pollution episodes then the ratio might stay the same therefore providing no valuable information. I would plot the SOA to OA as an alternative option or the SOA alone.

Figure 4: The data are really hard to observe. Please change colors and increase font size.

Figure 7: The graph is not clear. In the main text, the authors discuss that the daily maximum of SOA occurs when RH is greater than 70% in both cities. The RH is higher than 70% all the time. The time of the day is up to 24 hours and not 25. The markers and boxes for (c) are not discussed whether they represent the left or right axis.

Specific Comments

Line 34: Please elaborate more

Line 39: Please define generally with a statistical value that has meaning.

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Line 91: Please elaborate more on the "purer condensed organics" for non-experts.

Line 99: "neglect" instead of "neglected".

Line 99: Please elaborate more on 1).

Line 109: The sentence is missing a verb.

Line 128-131: The sentence is hard to read. Please rephrase.

Line 138: Which region?

Line 163: Don't change a line. Also, why acidic conditions? Please, elaborate more. Why is the reactive uptake of dicarbonyls, IEPOX and MAE in the "non-volatile" category?

Line 164: change to "was mostly"

Line 165: Please elaborate more on the non-ideality calculation of the organic-water mixture for non-experts.

Line 170: Is this the absorbing organic phase?

Line 196: Change to "as water condenses".

Line 200: Please elaborate more on the "Kelvin effect neglected" for non-experts.

Line 204: Change to "can be estimated".

Line 242: Observations in 8 sub-regions of the domain during which period?

Line 251: No significant improvements observed when applying the above additions means that the model is still missing a significant pathway to SOA formation, especially since OA in both seasons are dominated by SOA based on observations. This should be discussed in detail and in the context of previous studies and findings from AMS measurements in China.

Line 258: Does it capture the observed diurnal variation? What is the R2 or R of

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the timeseries of the modeled to observed values? What is the ratio of the two? In many cases, it seems that the difference is higher than a factor of 4. Is that a usual discrepancy? If so, how is much is it improved when incorporating the detailed SOA models?

Line 259: It would be great if “better” was described with statistical terminology. A way to describe the data and the comparison to modeled values would be to generate box and whiskers of the ratio of observations to modeled values for non-polluted and polluted days, respectively.

Line 262-263: POA is not the primary contributor to OA in Beijing in winter. Many studies show that SOA is the major contributor and the path towards SOA formation is currently unknown and strongly dependent on LWC in the particles. Aging of POA not treated in the model is not guaranteed to be the main source of SOA.

Line 280: Here only one season is provided in terms of timeseries comparison of the model and obs. Please provide both seasons.

Line 285: Figure S5 shows the anthropogenic SOA and not the dicarbonyl SOA. Please separate the contributions and discuss them in the main text. Identifying the contribution of different compounds to SOA formation in China would be of great interest to the scientific community.

Line 312: What about particulate nitrate?

Line 380: RH is higher than 70% all the time. What is the meaning of this sentence?

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