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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Simulation of SOA Formation from the Photooxidation of Monoalkylbenzenes in the Presence of Aqueous Aerosols Containing Electrolytes under Various NO_X Levels" *by* Chufan Zhou et al.

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Review of:

Simulation of SOA Formation from the Photooxidation of Monoalkylbenzenes in the Presence of Aqueous Aerosols Containing Electrolytes under Various NOx Levels.

1 General Comments

The manuscript by Zhou, Jang, and Yu present an improvement to the Unified Partitioning-Aerosol Phase Reaction (UNIPAR) model. The authors added an age-driven mass-based stoichiometric coefficient (α_i), to predict the temporal evolution of the aerosol system. They compare the new UNIPAR model to experiments conducted in the UF APHOR chambers.

The model improvement and experiments focused on aromatic molecules, specifically toluene, ethylbenzene, and n-propylbenzene. They used both seeded and non-seeded ammonium sulfate experiments as well as, wet vs. dry seeds. The updated UNIPAR model showed remarkably good agreement when a dynamic α_i was included in the model.

The manuscript is suited for Atmospheric Chemistry and Physics and is of interest to the community. It is well written and highlights essential insights into the partitioning and chemical reactions in multiphase aerosol particles. I have a minor comment regarding the dynamic α_i, and a few line comments. With these minor concerns addressed, I would recommend this manuscript for publication.

2 Specific: Dynamic α_i

I understand the mass-based stoichiometric coefficient (α_i), has to be dynamic to capture the full evolution of the aerosol mass. It is not clear on page 5 line 7, if the dynamic reconstruction is a fit to smog chamber data or not. Section 3.1 reads as if α_i was fitted at the beginning and ending conditions of the experiment. Then assuming that is correct, does α_i have any value other than a free parameter?

Since α_i was the major factor that brought the experiments and model into an agreement, is this fit general for the atmosphere or system specific?

3 Line Comments

- Page 1 line 13: "applied to estimate" would be clearer if changed to "used to estimate"
- Page 1 line 19: Shouldn't the importance of electrolytes over NOx or α_i, be expected or is this new insight?
- Page 1 line 21 and Page 11 line 14: "presence of wet electrolytic seeds" is this mainly the salting-in effect (and not chemical reactions) that causes the increase in SOA mass? From, Figure 7 the small fraction of OM_{AR} in A-D seems to suggest that is the case. Have you ran simulations at higher RHs, say 90%?
- Page 4 line 10: There are theoretical calculations to include in the support the assumption of phase separation. See Zuend, A. and Seinfeld, J. H.: Modeling the gas-particle partitioning of secondary organic aerosol: The importance of liquid-liquid phase separation, Atmos. Chem. Phys., 12(9), 3857–3882, doi:10.5194/acp-12-3857-2012, 2012.
- Page 5 line 26: How did you settle on this formula for the activity coefficients? I suggest adding that discussion to the SI.
- Page 11 Line 3: "RH is insignificant" only at these experimental conditions. Maybe change to "RH is insignificant for our experiments, discussed in Section 4.2."

- Figure 5: I find the figure's y-axis labels a bit cramped. Add a little more white space between the three panels to improve readability.

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