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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.

Anonymous Referee #2

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General Comments

This manuscript describes high-quality modeling efforts simulating a series of sunlit chamber experiments on toluene, ethylbenzene, and propylbenzene oxidation. The chamber experiments were conducted at varying RH levels so that the inorganic phase of aerosol would be liquid or solid at different points. NOx levels were also varied from experiment to experiment. The UNIPAR model was extended by the introduction of 6 reactivity bins within each volatility bin, along with separate treatment for glyoxal, methylglyoxal, and isoprene epoxidiol products. Futhermore, the mass-based stoichiometric coefficients of products were allowed to evolve between coefficients measured on fresh aerosol to those measured on aged aerosol. With these extensions, the model was able to simulate chamber data closely, while allowing the authors to compare the relative importance of environmental factors on SOA yields. They conclude that for monoalkylbenzene oxidation systems, the presence of an aqueous aerosol phase has a larger positive effect on SOA yields that switching from high NOx to low NOx conditions. This work will be of interest to a broad audience of scientists with interests in particulate air pollution and its mitigation.

Specific Comments

It is unclear which experiments were conducted in sunlight, and how this important factor affected the results. The paper mentions that the sunlight from one experiment performed near summer solstice was used in gas-phase simulations, apparently for all experiments, even those conducted in mid-winter. Were all experiments performed on clear days? How might using more intense sunlight in simulations of winter experiments affect the uncertainties of the results?

p. 6 line 10: Was oligomerization in both the organic phase and the aqueous (inorganic) phase based on self-dimerization of individual products, or lumped products? In other words, were cross-reactions possible between molecules lumped into a single bin?

p. 10 line 32: The authors identify a large temperature effect on SOA yields, as seen in other studies. However, the authors are uniquely positioned to identify whether this effect is due only to partitioning, as typically assumed, or is also due to temperature-dependent reactions that either destroy condensable species or produce other species that hinder gas-to-particle transfers. Partitioning seems to be such a minor SOA source in this study that it is surprising that the observed temperature effects are so pronounced. Could the authors probe the cause of the temperature effect?

In Figure 5, dialkyl organosulfates (diOS) concentrations seem to track ammonium concentrations. In one experiment, the authors comment that diOS formation ceases when the aerosol effloresces. Is there any causative relationship between diOS and ammonium concentrations in wet aerosol?

Figure 7 implies that in most experiments, aqueous-phase SOA production is much greater than SOA production via traditional partitioning mechanisms, but the authors don't seem to make this comparison or comment on it. Is it a fair comparison?

Figure S1 indicates that ozone is generated too quickly in the model, sometimes by a factor of 2 or 3. Can the authors comment on the implications of this overprediction? Is it related to the "artificial OH radicals" added to the model in certain experiments?

Technical Corrections

P. 2 line 5: Unclear comparison: " . . . fewer global emissions" that what?

p. 2 line 11: When the authors refer to "regional weather" do they really mean climate change?

p. 4 line 9: unclear comparison with literature: What system was "the reported value of 2" measured for? Is it a toluene oxidation study?

p. 6 line 18: another unclear comparison with literature: What system was "the reported value of 1.4 g/cm3" measured for?

p. 7 line 2: It appears that "irreversibility and nonvolatility" should be "irreversibly formed and nonvolatile".

p. 9 line 12: The meaning of the phrase "contributed to" is unclear in this sentence.

Interactive comment on Atmos. Chem. Phys. Discuss., https://doi.org/10.5194/acp-2018-963, 2018.