

Atmos. Chem. Phys. Discuss., referee comment RC1
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Comment on acp-2021-560

Anonymous Referee #1

Referee comment on "Synergetic effect of NH₃ and NO_x on the production and optical absorption of secondary organic aerosol formation from toluene photooxidation" by Shijie Liu et al., Atmos. Chem. Phys. Discuss., <https://doi.org/10.5194/acp-2021-560-RC1>, 2021

The script by Liu et al. reported synergetic effects of NH₃ and NO_x on toluene SOA production, chemical composition, and optical properties. Though experiment was not well designed nor some important information (experiment repetition, photon-flux, OH radical exposure, details in wall-loss correction, etc.) on chamber operation was provided, their results are interesting and important if all their speculations on chemical results were reliable based on simple AMS measurement. More chemical information on molecular levels and proper reaction pathways should be provided to verify the discussion. Besides, the authors should go through script carefully to check all the values and units. Overall, the decision is Major revision and the authors should address all the comments.

Specific comments:

- Line 107: "participate"
- Line 148: Particle wall loss rate is constrained by many factors, including particle size, chemical composition, and wall environment. You can surely use standard aerosols to derive a simple wall loss rate for ensemble particles in the chamber, but detailed information concerning the loss-rate should be provided and also discuss the feasibility to apply one rate to correct all experiments with different environments.
- In method description, what was the shape of your chamber? how do you control the chamber temperature when the whole teflon bag in operation was sealed in light box? And what is the light transition efficiency of your teflon bag? How to make sure the chemicals were eventually distributed in the chamber?
- What was the general OH radical concentration throughout each experiment? Did you quantify the OH radical exposure to ambient environment? Was it atmospheric environmental relevant for toluene photooxidation?
- Line 163: "NO_x (.....) or/and NH₃"
- Line 169: delete "present"
- Line 176: SMPS classifies electrical mobility size of particles.
- Line 180: Toluene SOA density shall be variant in response to different ageing degree and presence of NO_x or NH₃.
- Line 203: commonly W-mode was suggested to derive elemental ratio of organics from AMS results.
- Line 214: is "46.2 mm PTFE filter"?

- Line 215: what was the extraction efficiency? In presence of NO_x/NH₃, inorganics shall form along with toluene SOA. Did you consider the salt influence on the extract absorption? and also interference on AMS characterization of organic fractions? It should be noted that ammonium nitrate has interference on AMS ionization, f44 signal and associated elemental ratios.
- Line 229: how did you quantify methanol-soluble organic carbon in clear methanol solution? if MAC was calculated on the basis of organic carbon, the unit of M should be μg OC m⁻³.
- In experiments, did you feed air to the chamber during monitoring and sampling? If so, did you consider the dilution effect on your final results on SOA concentration? How many times you repeated each test?
- Line 233: change "during" to "on"
- Line 255: change to "this may at least partly explain....."
- Line 266-267: confusing, make the statement clear
- Line 275: in current toluene photooxidation with NO_x and NH₃ presence, nitrogen content is significant enough to be considered in carbon oxidation state calculation. The simplified OSc may be biased in chemical feature description of toluene SOA.
- Line 291: delete "toward", change to "continuing increase of SOA and its OSc"
- Line 284-300: time-profile of SOA mass concentration from UV on till end of experiment was needed to support your speculation of OSc changes. Besides, Organic (C_xH_y⁺, C_xH_yO⁺, C_xH_yO_i⁺, etc.) and inorganic contribution over the course of each test should be provided. Can you tell at what proper time OH radical was totally consumed in the chamber since UV on?
- Line 308: confusing. Ammonium salt offsets what?
- Why not use practical m/z-43 (C₂H₃O⁺) and m/z-44 (CO₂⁺) mass concentration changes to describe proper reaction pathways in toluene photooxidation? Mass fraction can only tell relative change.
- In tracking Hi-NOA and LO-NOA via PMF, have you ever considered application of some characteristic fragments indicating products by homogeneous acid-base reactions and heterogeneous Maillard reactions to verify your hypothesis? Molecular analysis by HRMS is most reliable compared to AMS derived results.
- Line 439: why dose Lo-NOA have higher N/C ratio? 0.062 vs. 0.29 for Ho-NOA vs. Lo-NOA?
- Line 449: how did you count the values of N/C ratio and percentage? Check all the values in the script carefully. 0.0404 and 0.216 accounts for 65% and 35 %, respectively?
- SOA concentrations have been summarized in Table 1, Figure 1 is not necessary, remove it. Besides, it is suggested to add photon flux and OH radical concentration information in Table 1.
- Redraw Figure 3, make it clearer. Suggest to add time information to trace time-profile of f43-f44
- Make clear statement of specific time for formation and stable stage of SOA in Figure 4, is it stable minus initial stage? Explain the presence of nitrogen-bearing fragments in Experiment 1.
- Present error and statistic results in Figure 5.
- Keep axis label and legend consistent in Figure 6.

Please also note the supplement to this comment:

<https://acp.copernicus.org/preprints/acp-2021-560/acp-2021-560-RC1-supplement.pdf>