

Interactive comment on “Chemical insights, explicit chemistry and yields of secondary organic aerosol from methylglyoxal and glyoxal” by Y. B. Lim et al.

Anonymous Referee #2

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General Comments

This work by Lim et al. describes a model for SOA formation from methyl glyoxal through multiphase processing. The authors developed explicit aqueous-phase OH oxidation mechanisms for acetic acid and methyl glyoxal. They validate these mechanisms against laboratory oxidation experiments, including a correction factor for H₂O₂ absorption of light. The mechanisms are then incorporated in their explicit glyoxal SOA model, and use it to simulate SOA formation under cloud water and aerosol water conditions. Since the mechanisms are explicit, they are able to determine product yield and which products dominate under which concentration conditions. They find that at low

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precursor concentrations, organic acids, specifically oxalic and pyruvic acid, dominate the products. At higher precursor concentrations, radical-initiated oligomer products dominate. This work presents a nice increase in our molecular-level understanding of aqueous-phase SOA formation. I think that this paper is suitable for publication in ACP after addressing the minor comments below.

Specific Comments

Page 7, line 12: Is there a reason the authors allowed the path length to vary while keeping the literature extinction coefficient, rather than keeping the known path length and allowing the extinction coefficient (which might have larger relative error bars than the path length) to vary?

Page 8, line 30: Can the authors give examples of precursors and conditions that are relevant for batch reactions vs CSTR reactions?

Page 10, line 8: Is there a reason CSTR reactions do not go above 10⁻⁴ M initial glyoxal or methyl glyoxal concentration?

Page 15, line 16: Even if the authors did not identify the compounds responsible for light absorption, did they observe a color change in their solutions?

Page 18, line 8: Can the authors quantify “substantial”, especially as from glyoxal, from methyl glyoxal, and from other compounds?

Can the authors comment on how the product chemical composition and distribution might change if chemistry with inorganics is allowed, as is likely in real aerosols with often contain quantities of ammonium sulfate and/or ammonium nitrate?

Technical Corrections

Page 3, line 18: b in “based” should not be capitalized.

Page 4, line 9: Perhaps use “unit mass resolution electrospray ionization. . .”

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Page 4, line 14: Reference for the triiodide method?

Page 6, line 21: Do the authors mean "Specifically" rather than "Specially"?

Page 11, line 11: "...faster than abstraction..." rather than "... faster that abstraction..."

Page 11, line 25: I believe a tertiary carbon means that it is covalently bonded to three other carbon atoms (which do not exist in either glyoxal or methyl glyoxal). Perhaps the authors could change the wording to "triply substituted carbon" or something similar to indicate they mean carbons bound to three non-H atoms?

Page 13, line 9: "... to our knowledge..." rather than "... in our knowledge..."

Page 15, line 2: "... slower rate than the literature value..." rather than "... slower rate that the literature value..."

Page 15, line 23: "Further work is needed to investigate this hypothesis." rather than the current concluding sentence.

Page 17, line 26: OH radicals rather than OH radical

Interactive comment on Atmos. Chem. Phys. Discuss., 13, 4687, 2013.