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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Investigative modeling of new pathways for secondary organic aerosol formation" *by* B. K. Pun and C. Seigneur

Anonymous Referee #1

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Review of MS-NR: acpd-2006-0372

This paper describes some exploratory 0D modeling of SOA formation. Treatment of SOA is based on recent literature (lab and ambient studies) as well as chemical analogy. There is recent evidence that current SOA model treatments do not sufficiently/accurately describe ambient SOA formation. The study is timely, thorough and explores a topic in atmospheric chemistry which is fraught with uncertainties. The authors highlight the most sensitive parameters of their scheme and suggest avenues for further research. This manuscript is appropriate for publication in ACP, however I find that the manuscript is somewhat disjointed. The reader would greatly benefit from a clearer road map and indications early in the text of which topics will be re-visited and which sensitivities explored.

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Specific Comments

The abstract should indicate that this study employs a 0D or box model

p.4: Liggio et al. [2005] show that the Henry's law constant 3.6x10ˆ5 M/atm produced insignificant aerosol-phase glyoxal. A reader familiar with this work will wonder why you chose to include glyoxal in this study, it should be clearly stated that you expect SOA formation from glyoxal ONLY as a result of oligomerization (as born out by Section 5.1)

p. 6: Since the Martin-Reviejo and Wirtz [2005] study was used to constrain benzene yields, it would helpful to see if the 0D model reproduces the experimental results obtained by those authors under varying initial conditions and as a function of time (for example comparing model with Figures 5, 7 and/or 8 of that paper).

p. 9: When discussing the 2nd isoprene mechanism, the authors fail to reference Table 2b. Section 4.1 is lengthy and occasionally hard to follow. A clearer overall description of how oligomerization is to be treated is required up-front.

p.14: The enthalpy of vaporization used requires a reference or justification.

p. 16: The description of Table 3 is confusing. The abbreviations AERO and AER should be introduced in previous paragraph. The fraction of each condensable that is subject to oligomerization (ie aldehyde) should be included in the table.

Table 4: A footnote should indicate that the corresponding parameters for benzene and isoprene can be found in Tables 1 and 2.

Table 5: Include the standard conditions pH and LWC in the heading (appear to be 3 and 50 ug/m3 given glyoxal product listed)

Section 5: I suggest that the authors quantify the overall effect of including oligomerization for all precursors in terms of total yield (as a function of pH) and discuss which SOA precursor class is most enhanced by this additional mechanism. This is commonly not treated in models and would seem a key result of this work.

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Figure 4 is never referenced in the text. The “high LWC” and “high POC” labels need to be explained in the caption.

Interactive comment on Atmos. Chem. Phys. Discuss., 7, 203, 2007.