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

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In this manuscript, a number of relatively recent developments from laboratory and ambient measurements of secondary organic aerosol (SOA) are modeled. Contributions to organic aerosol by benzene oxidation, isoprene oxidation, and oligomer-forming reactions are examined, and sensitivity of SOA formation to characteristics of background aerosol (primary organic aerosol, liquid water content, and pH) is investigated. Since (a) "new" SOA precursors such as benzene and isoprene have not been included in most models to date, (b) there is no established treatment of oligomer-forming reactions in models of atmospheric SOA production, and (c) models consistently underestimate atmospheric loadings of organic aerosol, this work is extremely important and timely. However the paper is a bit hard to follow, largely because of all the new approaches introduced, and it is not always clear that the approaches chosen are

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the most appropriate. The paper would be improved substantially if the treatments of the various SOA-forming systems (benzene, isoprene, oligomer formation) were made more consistent with one another (or, at the very least, explained in greater detail), and if model results were compared with laboratory data. Once these points (described below) are addressed, this manuscript will be suitable for publication in ACP.

1) Benzene, isoprene, and oligomerization all receive separate treatments, but this seems unnecessary. A major product of benzene oxidation is glyoxal (and similar ring-opening products); a major product of isoprene oxidation is methylglyoxal. Both dialdehydes are generally believed to contribute to SOA via oligomerization (at least at high RH). It is not clear why they require different treatments, which are also distinct from the treatment that other oligomerizing aldehydes receive. Is there any way to represent these three related systems using a single framework for partitioning?

Of specific concern is glyoxal and methylglyoxal; the two are extremely similar structurally (differing by only a CH2 group) and yet in this manuscript their partitioning involves fundamentally different physics (Henry's Law vs. APR). It would seem methylglyoxal, a water-soluble organic, should be well-described by a Henry's Law treatment (the same could be said for the other 2nd-generation isoprene products).

2) Given that the various systems examined in this work are generally poorly understood, and this work represents one of the first attempts to describe them within a model, it would be extremely useful to test these new modeling approaches against observations. This strikes me as an important step to take prior to the sensitivity studies (which are also very useful), as much could be learned about the various systems. For example:

- how well does the APR approach reproduce the Kroll et al (2005) or Dommen et al (2006) chamber isoprene data?

- how well does the approach towards benzene oxidation (with glyoxal partitioning) reproduce the Martin-Reviejo and Wirtz (2005) data?

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- there is substantial evidence that aldehydes undergo oligomerization in the presence of ammonium sulfate seed; how well does this treatment of oligomerization reproduce chamber data from terpene or aromatic oxidation (from which aldehydes are major products)? The acidity-dependent studies of Jang et al or Gao et al (2004) may be particularly useful for testing the predicted pH dependence.

Making each one of these comparisons is probably not necessary; but some comparison with laboratory data would serve as an excellent diagnostic for the appropriateness of the various approaches towards partitioning (APR, Henry's Law, Kp) described in this work.

3) For context, in the sensitivity studies, it would be useful if typical values of LWC and pH were given for both atmospheric and chamber conditions, preferably with citations.

4) The treatment of oligomerization (section 4.1) is quite hard to follow, and a general explanation of the overall approach used would be helpful.

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

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