**Atmospheric
Chemistry
and Physics
Discussions**

Interactive comment on "Global mechanistic model of SOA formation: effects of different chemical mechanisms" *by* G. Lin et al.

Anonymous Referee #3

Received and published: 11 November 2011

The paper "Global mechanistic model of SOA formation: effects of different chemical mechanisms" by Lin et al. explores the impacts recent developments in our understanding of SOA formation using a global model. Overall, I think this is a useful study, and the paper is generally clear and well written. I wish the authors would be a bit more careful with regards to how they describe model performance relative to the observations (no need to oversell, it's OK if there is more work to be done). Also, I think they could make their manuscript more important by digging a bit deeper into the implications of when and where their model improved agreement with observations, so as to posit some conclusions regarding which mechanisms may or may not dominate in the atmosphere. The introduction includes a fairly broad description of recent history of SOA, which, although not entirely necessary, I think is nice to have. At the rate at which this field moves, the authors should check for more recent SOA modeling works

Full Screen / Esc

Printer-friendly Version

Interactive Discussion

Discussion Paper

that have been published since the time they submitted their manuscript. Overall, I recommend this work for publication after the following issues are addressed.

(p.s. So as not to be biased, I have written this without looking over other reviews that have been posted, so I apologize if there is overlap).

1 Comments

(format: page.line)

- The title just doesn't read very well, and I'm not sure it's even grammatically correct. Can you refer to "a model"? or eliminate the colon and use the word mechanism only once? Colon's in article titles can almost always be eliminated if the title is better crafted. Can the type of mechanisms being considered be mentioned? For example, "Modeling the impacts of aqueous aerosol production, organic nitrates and peroxides on global SOA distributions" would be much more informative.

- 49: I think it is worth pointing out that recent modeling studies of urban SOA can even overestimate observed concentrations (Dzepina et al., ES&T. 2011; Hodzic et al., ACP, 10, 5491 – 5514, 2010), or at least come much closer (Li et al., ACP, 11, 3789 – 3809, 2011). Maybe that's a point to be brought up more on page 51, in which case you may want to refer to the studies in this paragraph as related to "traditional" SOA, or SOA from absorptive partitioning.

- 51.1 : Citation of Chung and Seinfeld here seems out of place, as that study pre-dated inclusion of SOA from isoprene. Also, Henze 2008 addresses aromatics (Henze 2006 deals with isoprene).

Interactive Comment

Full Screen / Esc

Printer-friendly Version

Interactive Discussion

Discussion Paper

- 53: This model resolution seems very coarse given the sparsity of data with which to compare. Can you comment on whether or not this leads to underestimates of SOA, and if so, by how much?

- 56: I think it's misleading to refer to the absorptive partitioning description of SOA as "non-evaporative". If you remove the surrogate secondary gas-phase species from such models, the SOA will evaporate.

- 57.18: Wasn't this work of Song 2007 on very fresh particles, with a very un-oxygenated organic substrate? Interesting, but how relevant as actual SOA substrate likely to much more aged?

- 58.4: This is not strictly correct. The two-product model assumes that the final yields in chamber data can be fit using surrogate species, which are place-holders for any number of oxidation steps in the gas-phase (Ng et al., 2006).

- 58.10: Also not strictly correct, as many of the more recent (post 2005) two product models are fit to yield data in NO_x free conditions.

- 58.17: I think the justification for the choice of model could be made stronger. Just recognizing that it is explicit seems like a weaker argument than, say, mentioning how such explicit representation leads to analysis that would not otherwise be possible with more empirical models.

- 58.25: Use a list format.

- 61: The subject of reversible vs irreversible uptake usually compares Kroll (2005) to Liggio (2005). The former was a long enough experiment to assess an equilibrium state, while the latter had the experimental setup necessary to assess kinetics. So these works aren't at odds as much as they are measuring different things.

- 65.16: Can references be provided for these sources?

- 66: It's not clear how evolution of the aerosol size distribution is being treated, if at all, or if the model only tracks aerosol partitioning.

- 68.6: It could be useful to briefly recap the simulation setups here.

- Should results from Fu 2008 be included in Table 5?

- 73: The statistical assessment could use some work. I think an additional useful metric would be a correlation coefficient or coefficient of regression. The NMBs, by themselves, don't reflect the fact that there is a lot of variability in the data that is not captured by the model. Also, it would probably be best to take the average of the IMPROVE data in grid boxes where there are multiple data points.

- 73.15: This seems out of place. Shouldn't this source of SOA be addressed earlier in the work where the model's treatment of SOA formation are discussed?

- 75.22: Might they also just deposit, rather than evaporate?

- 75.27: But does introduction of the mechanism make the urban comparison worse?

- 77: So overall, it seem that the model is getting large global burdens, but for the wrong reason?

- 79.6: reiterate here how they compared.

- 79.14: yet most of the enhancement you are seeing from POA is from POA from biomass burning?

- 79.27: The comments here about estimates of future SOA values seems out of place. Also, there are other modeling studies which show that owing to a balance of effects, the net impact on SOA is close to zero.

- 80.23: I think the agreement is a long way from being "close". For example, the model has no predictive skill compared to the EMEP observations.

- 81: Can the authors posit any broader conclusions here regarding mechanisms? In other words, what can we learn from the fact that the model overestimated in some places but underestimated in others? Does this help rule out / support any particular mechanism?

2 Corrections

- 50.13: Slowik 2011, not 2010?

- 51.1: Chung. A few other places the same typo.

- Surratt 2010 listed twice.

- 53: I think it's more proper to cite Ito et al. than to name the mechanism as Ito mechanism.

- 56: Peeters and Mueller (2010) missing from Bibliography.

- 57.6: Change K to K_i. Also, C^* needs a species index i.

- 57.12: Why say "assume"? Isn't this just a definition?

- 58.9: are built

- 66.14: Zhang 2000 not in Bibliography

- 66.14: Zhang 2000 not in Bibliography

- 78.23: the explicit . . . the 2-product → an explicit . . . a 2-product

Interactive comment on Atmos. Chem. Phys. Discuss., 11, 26347, 2011.

Full Screen / Esc

Printer-friendly Version

Interactive Discussion

Discussion Paper