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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Understanding the impact of recent advances in isoprene photooxidation on simulations of regional air quality" *by* Y. Xie et al.

Anonymous Referee #1

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Xie et al present a series of model simulations which assess the improvements of using an updated isoprene oxidation relative to the base isoprene mechanism used in their CMAQ model. They compare the model simulated fields of ozone and ozone precursors to a range of observations made over the South Eastern USA as part of the INTEX-NA/ICARTT campaigns owing to the fact that this is a region where one would imagine there exist string links between isoprene photooxidation and air quality. The convincingly show that the updated isoprene photochemical mechanism leads to an improvement in the ability of the model to simulate the observed ozone precursors. They then perform a range of sensitivity simulations which aim to address long standing issues with isoprene photochemistry, most notable the yields, recycling efficiencies and

deposition sensitivity of the isoprene nitrates.

Although this is not the first study to focus on the role of isoprene photooxidation in this part of the US, or for that matter the first study to make use of the INTEX-NA/ICARRT observations to evaluate model simulated compounds, I feel that the authors have done a really great job with this manuscript and would recommend its publication in ACP following appropriate response to the following minor points.

1) Missing NOy. The authors demonstrate that the model in both simulations (and presumably all the sensitivity studies) simulates NOy which is lower than observed, but SAN's which is much higher. What are the likely reasons for this? One would imagine that NOy is dominated by HONO2, PAN and the (Sum)AN's.

2) Constraints on "global" importance of NO3+Isoprene as source of ISON. Its strikes me as interesting that the reaction between NO3 and isoprene should really have such a large role to play on the formation of isoprene nitrates given that not much isoprene is emitted/exists at night. Do the authors think this could be a (general) model artefact (I note that this result has been observed in other modelling studies) or is there any observational evidence for enhanced formation of ISON during the night?

3) Computational overheads. It would be interesting to know how much more demanding the IS simulations were relative to the base case.

Technical corrections.

The following corrections refer to the page and line numbers in the ACPD paper.

27180-16: Use lower case k for rate constant.

27181-27: Add reference to da Silva 2009.

27185-15: You may want to add a comma after "from isoprene" and after "(MACR)".

27188-18: Add reference to Archibald et al., 2010 (this was included in the ref list but I couldn't see it in the main text).

27189-9: Add reference to Orland and Tyndall, 2012.

References:

Archibald, A. T., et al. "Impacts of mechanistic changes on HOx formation and recycling in the oxidation of isoprene." Atmos. Chem. Phys 10.17 (2010): 8097-8118.

Orlando, John J., and Geoffrey S. Tyndall. "Laboratory studies of organic peroxy radical chemistry: an overview with emphasis on recent issues of atmospheric significance." Chemical Society Reviews (2012).

Silva, Gabriel da, Claire Graham, and Zhe-Fei Wang. "Unimolecular β-hydroxyperoxy radical decomposition with OH recycling in the photochemical oxidation of isoprene." Environmental science & technology 44.1 (2009): 250-256.

Interactive comment on Atmos. Chem. Phys. Discuss., 12, 27173, 2012.