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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Exploration of the influence of environmental conditions on secondary organic aerosol formation and organic species properties using explicit simulations: development of the VBS-GECKO parameterization" *by* Victor Lannuque et al.

Anonymous Referee #1

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This work develops a simplified VBS-GEcko parameterization determined by fitting a lumped set of volatility bins to the explicit Gecko_A framework. Optimizations are performed by defining design test criteria in terms of VOC precursor, NOx, photolysis etc. The ultimate objective is to implement VBS-Geck in 3D chemical transport models. Overall, the paper is well written.

While the goals and methodologies are well defined, the following points need to be

explained: 1. While VBS-Gecko is compared to Gecko_A, it's not clear how either of these compares to actual SOA observations. Simulating some lagrangian test cases from field measurements of SOA would have been helpful to understand the utility of these approaches. 2. A fixed set of yields are fit to different volatility bins in VBS-Gecko. But multigenerational aging e.g. functionalization/fragmentation reactions can change the VBS distributions, especially at longer timescales. Could use of fixed VBS-Gecko (which do not change with aging) yields be responsible for the differences with explicit Gecko-A shown in Figure 8? I understand that the fixed yields are supposed to represent a fit to the entire dynamic evolution, but errors could be larger at longer timescales. 3. Condensed phase SOA processes as oligomerization can also alter volatility distributions, molar mass etc. How does VBS-Gecko or Gecko-A account for dynamic changes in SOA properties due to condensed phase chemistry? 4. In Figure 2, why is the condensed mass of n-octadecane (red line) much higher than the other 2 precursors? Is this result supported by smog chamber measurements? 5. Mechanistically, why does maximum yield decrease as the number of methyl groups in aromatics increase? 6. The enthalpies of vaporization are assumed to be NOx-independent and only depend on volatility bins. However, volatility of SOA is NOx-dependent. See Xu et al. 2014. Could the authors comment on how NOx-dependent volatility affects their assumptions of SOA properties e.g. enthalpies of vaporizations and molar mass? 7. Why do terpene SOA yields show the strongest sensitivity to temperature and pre-existing organic aerosol mass? 8. I recommend adding references to some recent review papers in the context of challenges in SOA measurements and modeling in the Introduction e.g. (Ng et al. 2017, Shrivastava et al. 2017).

References:

Xu, L., Kollman, M. S., Song, C., Shilling, J. E. & Ng, N. L. Effects of NOx on the Volatility of Secondary Organic Aerosol from Isoprene Photooxidation. Environ. Sci. Technol. 48, 2253-2262, doi:10.1021/es404842g (2014).

Ng, N. L. et al. Nitrate radicals and biogenic volatile organic compounds: oxida-

tion, mechanisms, and organic aerosol. Atmos. Chem. Phys. 17, 2103-2162, doi:10.5194/acp-17-2103-2017 (2017).

Shrivastava, M. et al. Recent advances in understanding secondary organic aerosol: Implications for global climate forcing. Rev. Geophys. 55, 509-559, doi:10.1002/2016RG000540 (2017).

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