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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Modeling SOA formation from the oxidation of intermediate volatility n-alkanes" *by* B. Aumont et al.

Anonymous Referee #2

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Predicting SOA formation and evolution from various precursors is one of the most challenging issues in atmospheric chemistry. Aumont et al. explore the time evolution of organic compounds and behavior of SOA formation from the photooxidation of C8-C24 alkanes under different concentrations of preexisting organic aerosol concentrations using the explicit modeling framework GECKO-A. The dependence of SOA production on the parent hydrocarbon structure and the preexisting organic mass is also investigated. I recommend this paper to be published in ACP, with minor revisions.

Major comment:

My primary concern is that the simulations are conducted only under high NOx conditions. Reactions of RO2+HO2 and RO2+RO2 have been neglected. In the real atmosphere, however, RO2+NO, RO2+HO2 and RO2+RO2 will occur to some extent simultaneously, depending on the abundance of OH radicals, VOC, and NOx. Is it possible to simulate a scenario in which these three sets of reactions are retained in the mechanism? This will provide some indication of the validity of neglecting the radial-radical reactions under high NOx conditions.

Minor revisions:

P14452, L5: Instantaneously partitioning theory is employed in this model. The fraction of species i in the aerosol phase is a function of C* and total organic mass. Could the authors give an example to incorporate this equation into the 2-step solver for species i? I assume the authors use ODE equations in their codes.

P14452, L15: Could the authors give any references for using 250 g/mol as the average MOA?

P14456, L5: The simulation results show that organic nitrates account for $\geq$ 49% of the first-generation products. However, previous chamber experiments found that molar yields of alkyl nitrates from C5-C8 alkanes range from 10.5 – 22.6 % (Atkinson et al., 1995; Arey et al., 2001). Could the authors give an explanation for the high yields of nitrates? What is the stoichiometric molar ratio of organonitrates from RO2+NO reactions in the mechanism?

P14456, L7: There is a small amount of trifunctional species formed in the first generational products. How do the authors define "one generation"? It seems that there should be at most two functional groups produced upon the abstraction of one H atom from the parent hydrocarbon by an OH radical via the 1,5-H-atom shift isomerization. Could the authors give an example of trifunctional species and how they are formed?

P14457, L15: I noticed from Figure 2 (k) that there are some 3rd-generation products with vapor pressure ranging from 10ˆ-8 to 10ˆ-2 atm. After 6 generation of oxidation, they are all gone. What is the fate of these products?

P14459, L5: The maximum yield was observed after the consumption of the parent hydrocarbon here. Chamber experiments, however, showed that for some VOCs like isoprene, secondary organic mass is still able to accumulate even after the parent hydrocarbon is completely consumed (Ng et al., 2006). The simulation here indicates that the further oxidation of semi-volatile products in the gas phase does not contribute to the SOA yield after the parent hydrocarbon is fully consumed. Given the constant OH radical supply, which is 2*10ˆ7 moles cm-3 s-1, the remaining gas-phase products should still be able to react with OH radicals.

P14461, L1: Figure 6 shows the distribution of parent compound vs. species with smaller carbon skeletons in the OSC/C* space. Could the authors give an estimate in terms of the fraction of all the fragments in both gas and particle phase as a function of time?

References: Arey, J., Aschmann, S. M., Kwok, E. S. C., and Atkinson, R.: Alkyl nitrate, hydroxyalkyl nitrate, and hydroxycarbonyl formation from the NOx-air photooxidations of C5-C8 n-alkanes, J. Phys. Chem. A, 105, 1020-1027, 2001.

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