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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Application of the Statistical Oxidation Model (SOM) to secondary organic aerosol formation from photooxidation of C_{12} Alkanes" *by* C. D. Cappa et al.

Anonymous Referee #2

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The authors present the application of a semi-empirical model (the statistical oxidation model - SOM) to chamber observations during the photo-oxydation of 4 distinct C12 alkanes (2 acyclic and 2 cyclic alkanes) under high NOx and low NOx conditions. The model is based on a kinetic approach designed to describe the multigenerational oxidation of a given parent compound. The chemical scheme describes the progressive functionalization and fragmentation of the carbon backbone based on 6 adjustable parameters. A regression is performed to fit the time evolution of both the SOA mass concentration and the O/C ratio observed during chamber experiments. A good model/measurement agreement is obtained. The study shows that a semi-empirical kinetic approach might be an appropriate way to parameterize the complex chemistry

involved in SOA formation. The paper is clearly presented and well written. I recommend the publication of this paper in ACP. Below are few comments and suggestions that the authors may take into consideration for the production of a revised version of the manuscript.

Comments:

The quantitative data used in Fig. 2 are already given in Table 2 (p. 27100). Figure 2 (p. 27102) is therefore useless and can be removed. Moreover, the histograms in Fig. 2 can also be found in Fig. 8 and 9.

Figure 6 (p. 27106) is difficult to read. Fig. 6A includes a very large number of time profiles (more than 30). The "orange cluster" (Nc=8-12, No=3) seems to lump species having very distinct behaviors at the beginning of the simulation. Is there a good reason to lump in that "cluster" the Nc=12 species (i.e. functionalization pathway) with the Nc =8-11 (fragmentation pathways). Furthermore, the only species that can be unambiguously identified in Fig. 6B is the (Nc=12, No=2) species. It would be helpful to add more information in Fig. 6B to identify the major contributors to the SOA mass.

P27090 (section 5.1). The Fig. 6A suggests a direct link between "cluster" and generation number. If this is correct, it would be helpful to examine and discuss this link in section 5.1.

P27093, line 18-21. It is shown that a reasonable model/measurement agreement can be obtained even if one of the parameters (here cfrag) is constrained. Therefore, I expect that various combinations of the 6 adjustable parameters could provide simulation results fitting the experiments in a reasonable way (at least within the uncertainties of the experiments). Can such distinct sets of parameters be identified or, in other words, can the uncertainties be quantified for the 6 values provided in each optimized set? This might be a critical point to interpret the physical meaning of the 6 parameters obtained after the regression.

The results show fairly distinct values for the best sets of parameters shown in table 2. Can this variability be commented in the context of future application of the SOM approach? In particular, how could the SOM model be constrained for a mixing of parent compounds evolving under various conditions? Can a single set of parameters be used to describe various parent compounds? Is it for example possible to provide a unique set of parameters allowing a reasonable agreement for all the experiments used in this study under the low and/or the high NOx conditions.

Minor comments:

P27079, L25: 2-methyl undecane is not a “linear” structure. “Acyclic” (instead of linear) may be used to lump dodecane and 2-methyl undecane in the same subset.

P27079, L18: The authors may add 2 additional references directly related to the topic of the present paper (alkane oxidation) as examples of dynamic frameworks for the modeling of SOA formation: Jordan et al., Atmos. Env., 8015-8026, 2008; Aumont et al., ACP, 7577-7589, 2012.

Interactive comment on Atmos. Chem. Phys. Discuss., 12, 27077, 2012.