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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Mechanism reduction for the formation of secondary organic aerosol for integration into a 3-dimensional regional Air Quality Model: α-pinene oxidation system" *by* A. G. Xia et al.

Anonymous Referee #2

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This paper considers the systematic reduction of a detailed mechanism for alpha-pinene oxidation in the atmosphere (derived from the MCM), with the primary aim of generating a mechanism describing secondary organic aerosol (SOA) formation that can be used in a 3-D regional scale model. Five methods of mechanism reduction are considered, including four existing methods and a specifically developed linear lumping approach, yielding an overall reduction of a factor of 2.5 and a mechanism containing 125 species and about 350 reactions.

The paper considers a topic which is appropriate for ACP. It provides a clear and sys-

tematic account of the reduction methods and how they were applied to the example mechanism: and is certainly of sufficient merit and interest to be published. That said, I do have some comments about the broader applicability of the linear lumping approach to atmospheric organic chemistry mechanisms, and how the work described fits into the larger programme of work implied by the title. These are now outlined.

The gist of the linear lumping approach, as described, appears to be that species of similar reactivity, formed (in most cases) from the same class of reaction at the same oxidation "generation" can be lumped. In some cases (e.g., NAPINAOOH and NAPINBOOH) the lumping seems very sensible, as the species are isomers which have similar degradation chemistry. In other cases (e.g., C720NO3 and APINCNO3), a C7 species is being lumped with a C10 species and (as indicated) this must only be viable because the formation fluxes of each are small (i.e., the species derive from the most minor channel of the OH + alpha pinene reaction and from minor channels of RO2 + NO reactions within that channel). My feeling is that the approach as described can yield practical reductions only in relatively simple systems (e.g., chamber experiments with a single VOC), although it is noted that the reduction in the number of species here is only 7%. In full atmospheric mechanisms when there are many more emitted VOCs (from different sources with different speciations and temporal profiles), and many products can be formed from more than one precursor and at more than one generation of oxidation, I suspect that the fraction of species which can be lumped in this way will be much smaller and that the method may not be as practical.

The title of the paper suggests that the presented work is part of a much larger programme which will consider many other VOCs, some of which will make SOA. The current alpha-pinene subset includes 125 species, indicating that the full mechanism will be somewhat larger. Given the authors introductory statement indicating "the need for an accurate yet simple mechanism", perhaps some indication should be given on what level of simplicity is required for the target 3-D modelling activities, and on how the current works fits into the broader work programme implied by the title of the paper.

ACPD

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Interactive Comment

Despite these slightly negative comments (which I hope the authors can address), I reiterate that the information provided in this paper is valuable and publishable.

Interactive comment on Atmos. Chem. Phys. Discuss., 8, 13301, 2008.

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