

Interactive comment on “Modelling the evolution of organic carbon during its gas-phase tropospheric oxidation: development of an explicit model based on a self generating approach” by B. Aumont et al.

B. Aumont et al.

Received and published: 19 May 2005

We would like to thank the referee for the comments

Specific comments

> If no additional model work is available on a larger range of VOC (for example highly branched species), the abstract should remove the reference to “organic

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compounds” and replace this with a term that more accurately describes the class of compounds for which the generator is able to produce oxidation mechanisms.

The generator manages highly branched species as long as the species is an acyclic compound. The abstract will be modified to restrict VOC to acyclic species only (see also the reply to referee #1). The tests performed so far did not highlight problem for long chain species. However, performing truly explicit scheme for species having more than 8 carbons is extremely consumer of computing resources (CPU and memory). For example, on a 2.5 Ghz PC with 1 Gb memory, it took about a week to generate the scheme and a month to solve it time in a box model for 5 simulated days. However, performing fully explicit scheme for long chain species is not very relevant. Many intermediates have very similar structure and properties and some lumping could be performed, even to address scientific question directly linked to the evolution of organic matter in the troposphere.

> Some determination of the sensitivities of the model outputs to significant rate coefficients and branching ratios would be useful.

Performing sensitivity study is clearly one of the main goals of the generator. However, full exploration of the sensitivity of model results (e.g. ozone production, radical budgets, NO_x budget, secondary organic speciation and amounts, etc.) to inputs (rate constants, reaction pathways, physical and chemical environmental conditions, emissions, dilution, etc.) is beyond the scope of this first paper describing the generator. Clearly, additional studies (and publications) are planned to address the sensitivities in much greater detail.

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> *It would be useful to know the time differences on running the different models.*

Based on the conditions used for heptane simulation: the generator scheme requires 500 more time than MCMv3 chemical scheme and 20 000 more time than SAPRC99 scheme.

> *Here also some analysis of why the different approaches (generator, SAPRC99 and MCMv3) lead to the largest differences in some of the secondary products presented HCHO, methyl glyoxal and PANs would be useful, and what is different about the 2 examples given that leads to a larger discrepancy in HCHO for heptane than isoprene for the SAPRC99 code?*

The analysis of the discrepancies requires a discussion of the parameterization used in SAPRC99 and MCMv3. Although very interesting, this is beyond the scope of this study. The purpose of the comparison was just to check the generator provides chemical schemes that are consistent with other “reference” schemes (at least in term of O3, NOx, HOx, ...). See also reply to referee #1.

Technical corrections

The suggested corrections are performed in the revised version of the paper.

Interactive comment on Atmos. Chem. Phys. Discuss., 5, 703, 2005.

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