Atmos. Chem. Phys. Discuss., 5, S832–S835, 2005
www.atmos-chem-phys.org/acpd/5/S832/
European Geosciences Union

Atmospheric Chemistry and Physics Discussions

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

Generator

> For illustrating better the representation of the molecule structure in the programme, I would suggest to add a figure comparable to Figure 2.3 of

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Laval-Szopa (2003).

OK. Such a figure is added in the revised version.

> The authors should give some information about the representation of the functional groups by the "group vector": which functional groups can be represented, are there any restrictions?

The generator only uses empirical data (e.g. rate constants or SAR). The chemistry can therefore be generated only for molecule bearing functionalities already defined in the generator and for which kinetic data are available. An example of the functional groups known by the generator is given page 710, line 10. Three additional functional groups must be added to the list given page 710, namely alkene, ether, ester. We discuss more specifically this point in the revised manuscript (see reply to referee #1). There is no conceptual problem to add functional groups (e.g. halogen group) but the reactivity induced by this new functionality must obviously be parameterized in the generator.

> How easily a user can introduce new kinetic data to the data pool?

Kinetic data are all provided in files. It is straightforward to add new kinetic data or update these files. These files are simply read by the generator.

> Can the SAR data easily be updated? Is this update still easy if it requires not only updating numbers but also changing the type of equation?

No. SAR are directly introduced in the Fortran 77 code (no user interface) and a new subroutine must be written for each new SAR. However, the code has a highly modular structure and changing a SAR to another is fairly simple (but

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obviously requires some knowledge of Fortran).

> Can new reaction pathways be introduced to the generator? Can all this be done without touching the FORTRAN code?

No. Like the SAR above, rules for new reactions must be added directly into the code. In fact, additional reactions can easily be added as long as these reactions do not lead to new functional groups (see above).

> The authors should add some information addressing to these questions for giving the reader a better idea of the possibilities and restrictions of the generator.

See reply to referee #1 and #2. The manuscript is mostly devoted to presenting the benefit and the potential of the self- generating approach to address scientific questions. However, the questions above showed us the need to describe in details how the generator "works" in a report made available on the web. Such a report is under preparation.

> One last question: A recently published generator of Kirchner (Atmos. Environ. 39, 1143-1159, 2005) is available on the internet. Will the generator of Aumont et al. also be available for the scientific community?

We would be very pleased to share the generator with the scientific community. Nevertheless, the current version of the generator is clearly a research code. The user interface first needs major improvements.

Kinetic data

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Interactive Comment

> The treatment of R-OC(.)O radicals should be corrected.

See reply to referee #1.

> For the treatment of alkyl peroxy radical - acyl peroxy radical reactions I suggest to add the following reference: Villenave, E., R. Lesclaux, S. Seefeld and W.R. Stockwell, 1998: Kinetics and Atmospheric Implications of Peroxy Radical Cross Reactions Involving CH3C(O)O2 Radical, J. Geophys. Res., 103, 25273-25285.

OK. The reference is added in the revised manuscript.

> Differences by comparing several mechanisms may result from the representation of the species in the mechanism, from the considered reaction path ways and/or from the kinetic data base used for creating the mechanism. Evaluating the origin of differences ...

See reply to referee #2.

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