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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.

Anonymous Referee #3

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General Comments

The automatic generation of chemical mechanisms is an important tool for updating mechanisms, adapting them well to the specials issues of investigation and for investigating the sensitivity to different ways of mechanism reduction. This article illustrates the large amount of species and reactions resulting from the degradation of even fairly small VOCs, making it nearly impossible to develop complete degradations schemes without a tool like the presented generator. This articles deals with three main topics:

generator, kinetic data base, comparison of the model results to the results applying other mechanisms.

Generator

The description of the generator is rather poor. 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 Laval-Szopa (2003). In addition 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? An important application for generators of this kind results from the velocity with which mechanism can be updated by introducing new kinetic data. I miss some important information concerning the question how easily a user can introduce new kinetic data to the data pool? 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? Can new reaction path ways be introduced to the generator? Can all this be done without touching the FORTRAN code? 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. 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?

Kinetic data

According to the references given in the article the kinetic data are based on the most recently recommend values. As mentioned by referee #1, the treatment of R-OC(.)O radicals should be corrected. 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. Results

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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 is always very difficult, especially if the differences are mainly small as they are in this comparison. Nevertheless, it would be useful if the authors could state if there are some major differences either in the kinetic data base (SAPRC-99 is older, are there some major changes in rate constants?) or in the considered degradation pathways between these mechanisms.

Recommendation

I recommend to publish the article with minor revisions after including answers to the questions mentioned above (especially those concerning the generator).

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