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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Mainz Isoprene Mechanism 2 (MIM2): an isoprene oxidation mechanism for regional and global atmospheric modelling" *by* D. Taraborrelli et al.

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We thank Zhang (2008) for stimulating us to clarify and improve our manuscript.

We want first to address the main question raised, whether our mechanism is state-of-art or not.

The purpose of this study is to provide a reduced mechanism capable of including new experimental and theoretical results in 3D models in a meaningful way. In this regard, MIM2 is an important step towards the development of a state-of-art isoprene oxidation mechanism in 3D atmospheric models. Following on the comment by R. Zhang, we would like to try to show more clearly how this reduced mechanism we present serves this purpose. To do so, in the revised version of the manuscript we will

add a new section in which we will show the differences due to a modification of MIM2, directly including few very recent experimental results (which is not possible with more traditional reduced mechanisms like MIM):

1) elimination of the species MVKOH (1-hydroxybut-3-en-2-one), since Benkelberg et al. (Phys. Chem. Chem. Phys., 2000, 2, 4029-4039) found no evidence for its formation from isoprene oxidation.

2) implementation of the new degradation of methyl vinyl radical from MACR oxidation (Orlando et al., Geophys. Res. Lett., 1999, 26, 2191-2194).

3) adoption of the product yields for the first peroxy radicals of isoprene as recently determined by Paulot et al. (ACPD, 2008, 8, 14643-14716).

4) adoption of the corresponding (see point 3) alkyl nitrate yields from the RO2 + NO reactions.

5) inclusion of the new results on the RO2 + HO2 reactions for which OH has been found to often be a product (Dillon and Crowley, ACP, 2008, 8, 4877-4889).

We are afraid that Zhang (2008) might have missed the Electronic Supplement, in which we provided all the necessary kinetic documentation to make use of our mechanism. Concerning the mechanistic information for which MIM2 stands, it is the same as for MCM, for which extensive documentation in the literature has already been provided (Jenkin and Hayman (1995), Jenkin et al.(1997), Jenkin et al.(1998) and Saunders et al.(2003)).

Zhang (2008) indicates that we make an unsubstantiated statement:

"Our new mechanism is expected to substantially improve the results of atmospheric chemistry models by more accurately representing the interplay between atmospheric chemistry, transport and deposition, especially of nitrogen reservoir species."

We acknowledge that this statement can be misleading for the reader. In fact, this

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statement is more the expression of one of our long-term goals. Therefore, we will change the sentence at page 14034 lines 23-25 to

"Our new mechanism is expected to substantially improve the results of atmospheric chemistry models by representing many more intermediates, that are transported and deposited, which allows us to test model results with many more new measurements".

Interactive comment on Atmos. Chem. Phys. Discuss., 8, 14033, 2008.