Atmos. Chem. Phys. Discuss., 8, S6503–S6505, 2008
www.atmos-chem-phys-discuss.net/8/S6503/2008/

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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Received and published: 29 August 2008

In this paper the authors present an oxidation mechanism (MIM2) of intermediate size for isoprene. They suggest its suitability for simulations in regional and global atmospheric chemistry models, on the basis of comparisons with its earlier versions of the Mainz Isoprene Mechanism (MIM) and the Master Chemical Mechanism (MCM v3.1). However, there are several major deficiencies that cast doubt on the objective of this work, that is to improve the representation of tropospheric chemistry in regional and global models.

Because of its important implications in tropospheric chemistry, such as in the forma-

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tion of ozone and secondary organic aerosol, the kinetics and mechanism of isoprene oxidation have been a subject of numerous experimental and theoretical investigations. Recently, important progress has been made in experimental studies to quantify several key species in the reaction products (such as hydroxycarbonyls and organic nitrates), to probe the reaction intermediate species, and to determine the isomeric branching of isoprene oxidation. In addition, theoretical studies using quantum chemical calculations have further refined the kinetics and mechanism of the isoprene oxidation. However, few of those recent important studies have been discussed in this work. As such, it is difficult to evaluate whether the present mechanism accurately represents the state-of-art knowledge toward isoprene oxidation. It will be crucial to explicitly describe of which, if any, those recent developments in experimental and theoretical studies on isoprene chemistry have been incorporated in the present formulation.

Another glowing deficiency in this paper is the failure to present and document the kinetic and mechanistic information for which the MIM2 stands. Except in Fig. 2 that contains limited data regarding the isomeric branching of the OH-isoprene reactions, important rate constants, their pressure- and temperature- dependencies, product yields, and branching ratios are not provided in the paper. Furthermore, nothing is provided for the reactions of isoprene with ozone and NO3. Such omissions preclude possible adoption of their mechanism by other modelers. All of the kinetic and mechanistic data relevant to the present mechanism need to be clearly tabulated.

The statement that "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" is not substantiated. Other than comparisons with its earlier versions and MCM v3.1, there was not attempt made in this work to validate the present mechanism by comparisons with experimental chamber studies or results from field measurements.

For their mechanism to be of utility to the community, those above aspects need to be carefully addressed by the authors.

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

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