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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.

D. Taraborrelli et al.

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In their Short Comment, Dibble (2008) cites a large body of literature (of which we are aware), indicating that OH addition to isoprene occurs primarily at C1, and asserts that in the MCM (on which MIM2 is based), 50% of OH-addition occurs erroneously at C2. We believe this assertion to be mistaken. We wish to assure T.S. Dibble and other interested readers that the MCM indeed has 65.5% OH addition occurring at C1.

The MCM is not a totally explicit mechanism. Alkyl radicals resulting from OH addition to isoprene are assumed to react instantaneously with O2 forming peroxy radicals. Browsing the MCM website, it can be seen clearly that the peroxy radical isomers ISOPAO2 and ISOPBO2 derive from the OH-addition occurring at C1. They

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have the formulae HOCH2C(CH3)=CHCH2O2 and HOCH2CO2(CH3)CH=CH2, respectively. Summing their yields, one obtains 65.5%. This number has not changed since Jenkin et al. (1997) and it is still extremely close to the most accurate and recent estimate by Greenwald et al. (2007), being 67%. Moreover, this number is within the range of 56-72% of all of the recent estimates (Stevens et al(2000), Lei et al. (2001); Greenwald et al. (2007); Peeters et al. (2007))

To reiterate, we wish to make it clear that the MCM, as well as MIM2 (which is based on the MCM), neglects the alkyl peroxy radicals deriving from the OH-addition occurring at C2 and C3. This approximation is considered acceptable even in light of the above cited studies in which the yields of these peroxy radicals should be in the range 0-7%.

In the Electronic Supplementary Material we have provided extensive further information about MIM2, including all of the reactions and species formulae. Based on both of the two short comments submitted thus far, we suspect that this Supplementary Material may have been overlooked. With regards to the comment of Dibble (2008), in the Electronic Supplement it can be clearly seen that in MIM2 the peroxy radicals from OH-addition at C1 are represented by the species ISOPBO2 and LISOPACO2. The production and chemistry of ISOPBO2 are the same as in the MCM and LISOPACO2 is a lump of the MCM species ISOPAO2 and ISOPCO2.

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