

Interactive comment on “Protocol for the development of the Master Chemical Mechanism, MCM v3 (Part B): tropospheric degradation of aromatic volatile organic compounds” by M. E. Jenkin et al.

Anonymous Referee #2

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This paper describes improvements to the Master Chemical Mechanism. In particular it considers the treatment of the tropospheric degradation of aromatic volatile organic compounds. In a companion paper, the mechanisms for the degradation of other volatile organic compounds are updated. This brings the Master Chemical Mechanism to version number 3, and it has been constructed using work from the literature up to the beginning of 2001. The MCM is a near-explicit chemical mechanism describing the degradation of organic compounds important in tropospheric chemistry and is a very valuable tool for the atmospheric community. The value of such a mechanism can only be maintained if the input data are updated with the literature and so this paper and its

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companion are welcomed.

The mechanisms for the degradation of aromatic VOCs are complex and not fully understood, which creates difficulties in developing the degradation schemes. The authors have approached the problem systematically and have generated a protocol that makes the best use of current knowledge in this area. Photochemical Ozone Creation Potentials are calculated for the aromatic VOCs and compared with those produced from previous versions of the MCM. Significant differences are observed, and these can be rationalised in terms of improvements in the MCM. I have no substantive criticisms to make and the paper is well written, clearly referenced and virtually free of typographical errors. My opinion is that the paper is publishable in its present form. I have some very minor points to raise. In line 23 of page 1910, the hydroxycyclohexadienyl radical and its derivatives are described as existing in up to three canonical forms. I don't really think the radicals exist in these forms. Rather, the radical can be described as a combination of the canonical forms and the electron distribution is such that attack by O₂ can take place at up to three positions (although for the parent radical there are only two). In section 4.3.1, the heading is 'Rates of initiation..'. Should this not be 'Rate coefficients for initiation...'? In that section, line 8, 'The review of Calvert...'. On page 1914, line 13, I don't understand 'For aromatics containing alkyl groups which are not identical (e.g. 1,2,4-trimethylbenzene),...'. The methyl groups are identical. In sections 4.5.2 and 4.5.3, the 1,4 addition peroxy radical is assumed to behave as a normal peroxy radical, while a variety of reactions for the 1,2 addition peroxy are described. There is no explanation for why the 1,4 radicals are treated as simple peroxys.

Interactive comment on Atmos. Chem. Phys. Discuss., 2, 1905, 2002.

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