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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Development of a detailed chemical mechanism (MCMv3.1) for the atmospheric oxidation of aromatic hydrocarbons" *by* C. Bloss et al.

Anonymous Referee #1

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This high quality paper contains an important documentation of the most recent improvements of the MCM3 to MCM3.1. Continuous updates of mechanisms can be a very tedious work but they are necessary to be able to test our current knowledge. The possible improvements due to these updates should be tested by high quality measurements as shown in this paper. In this paper, recent literature on various degradation pathways of different aromatics has been used to update the Master chemical mechanism. A number of key compounds are measured to assess in some experiments if the model has improved. The results might seem somewhat frustrating. Mostly only slight improvements of the model measurement comparison are found and very big uncertainties remain nearly for all systems described. Some interesting suggestions are given at the end concerning which pathways might be wrong in the model.

More work with a close cooperation of model developing and high quality experiments is needed. As mentioned by the authors at the end, the measurement capabilities of oxygenated intermediates should be improved.

Specific comments:

- The number of key components measured seems to be a bit low. For these key components, it is not discussed enough how good the data quality is. Are the differences between model and measurements maybe also due to measurement uncertainty?? How good are the OH LIF measurements in comparison to OH derived from hydrocarbon decay (where applicable).

- At the very end, PTR-MS measurements are suggested. Are they really as valuable as suggested taking into account that they cannot unambiguously detect a compounds with the same mass? In addition there are also fragmentation issues.

- Page 5769: The measurement of which oxygenated intermediates would be crucial to better understand the dicussed systems?

- In Table 3, 'glyoxal' can hardly be read.

- The recent findings on polymerisation reactions within aerosols could be mentioned in the discussion. Kalberer et al. (2004, Science) have shown that some low and reactive molecular weight compounds as HCHO, glyxoal, methylglyoxal might be incorporated in the aerosol and are thus removed from the further oxidation chain in the gas phase.

Interactive comment on Atmos. Chem. Phys. Discuss., 4, 5733, 2004.

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Interactive Comment