

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

C. Bloss et al.

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We thank the referee for useful comments and have addressed them as follows

Specific comments: 1. 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).

The following text has been added to section 4.4: It is important to assess the statistical significance of the discrepancy between the measurements and the models. This has

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been done extensively in recent papers. Zador et al (2004) carried out a detailed statistical analysis for ethene photo-smog experiments, examining uncertainties in both models and measurements. Bloss et al (2003) made a careful comparison of the rate of decay of several aromatics and [OH] as measured by FAGE and found generally good agreement, within the combined uncertainty limits. It is clear that the discrepancies in ozone, OH and NO_x concentrations found in the present papers far exceed those expected on grounds of measurement and in model parameter uncertainties. Hamilton et al (2003) used GCxGC to search for the expected co-products of glyoxal and methyl glyoxal in toluene, but the yields were substantially below those predicted by the current mechanism.

2. 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 compound with the same mass? In addition there are also fragmentation issues.

This has been reworded:

Sensitive on-line techniques should be employed ... atmospheric levels. Proton-transfer-reaction mass spectrometry experiments, for example, should be useful, if targeted at specific compounds, where interferences can be eliminated.

3. Page 5769: The measurement of which oxygenated intermediates would be crucial to better understand the discussed systems?

Additional text has been added: ...in aromatic degradation. In particular, it is essential to identify quantitatively the co-products of glyoxal and methyl glyoxal in toluene oxidation. This is a demanding requirement, since the species formed are likely to be highly photochemically reactive.

4. In Table 3, glyoxal can hardly be read.

The table has been re-configured

5. The recent findings on polymerisation reactions within aerosols could be mentioned

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in the discussion. Kalberer et al. (2004, Science) have shown that some low and reactive molecular weight compounds as HCHO, glyoxal, methylglyoxal might be incorporated in the aerosol and are thus removed from the further oxidation chain in the gas phase.

The following text has been added to p 5765:

In the aromatic ...condensed gas phase (Kalberer et al, 2004). Because the aerosol yield ... only a small effect on the gas phase organic chemistry. This issue is discussed at greater length in the companion paper.

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

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