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Development of a detailed chemical mechanism (MCMv3.1) for the atmospheric oxidation of aromatic hydrocarbons

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Abstract. The Master Chemical Mechanism has been updated from MCMv3 to MCMv3.1 in order to take into account recent improvements in the understanding of aromatic photo-oxidation. Newly available kinetic and product data from the literature have been incorporated into the mechanism. In particular, the degradation mechanisms for hydroxyarenes have been revised following the observation of high yields of ring-retained products, and product studies of aromatic oxidation under relatively low NO_x conditions have provided new information on the branching ratios to first generation products. Experiments have been carried out at the European Photoreactor (EUPHORE) to investigate key subsets of the toluene system. These results have been used to test our understanding of toluene oxidation, and, where possible, refine the degradation mechanisms. The evaluation of MCMv3 and MCMv3.1 using data on benzene, toluene, *p*-xylene and 1,3,5-trimethylbenzene photosmog systems is described in a companion paper, and significant model shortcomings are identified. Ideas for additional modifications to the mechanisms, and for future experiments to further our knowledge of the details of aromatic photo-oxidation are discussed.

Final Revised Paper (PDF, 453 KB) Discussion Paper (ACPD)

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