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Evaluation of 1,3,5 trimethylbenzene degradation in the detailed tropospheric chemistry mechanism, MCMv3.1, using environmental chamber data.

A. Metzger (1), J. Dommen (1), K Gaeggeler (1), J. Duplissy (1), A.S.H. Prevot (1), U. Baltensperger (1)

(1) Laboratory of Atmospheric Chemistry, Paul Scherrer Institut, 5232 Villigen, Switzerland

The degradation mechanism of 1,3,5-trimethylbenzene as implemented in the Master Chemical Mechanism version 3.1 (MCM) was evaluated using environmental chamber data from the Paul Scherrer Institute and from chambers at the Statewide Air Pollution Research Center (SAPRC) at the University of California, which have been used in previous appraisals of the MCM.

The results show that the MCM provides a consistent description of the photo-oxidation of TMB/NOx mixtures for a range of initial VOC-NOx-ratios, but with a significant underestimation of the decay rate of TMB and thus underestimation of reactivity in the system. This is in strong contrast to the observed overestimation of ozone by the model. The results reveal a strong dependence of the model performance on the initial VOC-NO_x ratio. In all cases the agreement between the measurement and the simulation decreases firstly with decreasing VOC-NOx ratio and in addition with increasing precursor concentration.

Our results suggest that the discrepancy between model and measurement is not solely due to mechanistic uncertainties but rather due to external factors like wall effects. This is supported by the measurement of much higher nitrous acid (HONO) concentrations compared to simulations and expected from chamber characterization experiments. Adding an additional NO_2 dependent HONO formation the model performance is improved for all experiments. The source of the increased HONO formation rate is still unclear. It is shown that the observed overestimation of ozone is directly linked to

the NO_y chemistry.