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Evaluation of the degradation scheme of 1,3,5 trimethylbenzene using smog chamber data.

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Environmental chambers are a common tool to study atmospheric reactions under controlled conditions. Results can be used to evaluate chemical mechanisms. However, chamber effects like adsorption, desorption, decomposition and possible surface reactions of reactants and products on the chamber wall can lead to artifacts. Therefore, for the validation of the model these artifacts have to be taken into account.

More than 40 experiments studying the 1, 3, 5 trimethylbenzene /NO_x (/propene) chemistry with varying VOC/NO_x ratios were conducted at the PSI smog chamber. A set of different instruments including proton transfer reaction mass spectrometry (PTRMS) and ion-chromatography (IC) were used to follow the degradation of TMB and to identify major products.

Model simulations were performed with the Master Chemical Mechanism Version 3.1 (MCMv3.1) to simulate the progression of the gaseous reactants and their oxidation products. The comparison of the simulation with experimental data reveals several shortcomings. The TMB decay and the build up of some major products could not be satisfactory described by the model. Also the comparison for the inorganic species show major discrepancies. The simulated NO decay is about 60% slower than the measured one. The CO formation is finally over 100% higher than simulated by the MCM after 480 min. The predicted O3 maximum after 180 min is also nearly double of the measured concentration.

Therefore chamber dependent parameters (based on characterization experiments) were included into the mechanism to optimize model simulations. Additionally, con-

siderations regarding the radical budget were conducted to optimize simulations.