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Investigation of aromatic compound degradation under atmospheric conditions in the outdoor simulation chamber SAPHIR

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Ozone is produced in the lower troposphere by the OH-initiated photooxidation of volatile organic compounds in the presence of NO_x. Aromatic hydrocarbons from anthropogenic sources are a major contributor to the OH-reactivity and thus to ozone formation in urban areas [1]. Moreover, their degradation leads to formation of secondary organic aerosol. Aromatic compounds are therefore important trace constituents with regard to air quality.

We will present the results of photooxidation experiments which were conducted in the atmospheric simulation chamber SAPHIR at Forschungszentrum Jülich. The experiments were designed to investigate the degradation mechanisms of benzene and *p*-xylene, which are among the most abundant aromatics in urban air samples. Benzene and *p*-xylene were selected because they have high structural symmetry which limits the number of potential isomers of secondary products. The experiments were performed under low-NO_x-conditions ($\leq$ 2 ppb). SAPHIR was equipped with instruments for the measurement of the parent aromatics and their major oxidation products, OH radicals, important radical precursors (O_3, HONO, HCHO), photolysis frequencies and particulate matter.

As shown in previous studies, simulation chamber data from the photooxidation of aromatics cannot be explained satisfactorily with current photochemistry mechanisms. For example the MCMv3.1 tends to overestimate the ozone-concentration and to underestimate the OH-concentration [2]. In this study, we will contrast model calculations with experimental results to check if similar discrepancies can be observed in SAPHIR and how they can be resolved. Based on the results of this preparatory study, further simulation chamber experiments with special emphasis on the radical budget are scheduled in 2010.

References:

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