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Degradation studies of methacrolein at the atmosphere simulation chamber SAPHIR

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The degradation of methacrolein (MACR) induced by OH radicals, photolysis, ozonolysis, and NO_3 radicals was studied at the atmosphere simulation chamber SAPHIR at the Research Center Jülich. MACR is a main product of the photochemical isoprene degradation and is therefore of great importance for the tropospheric photochemical ozone production.

Measurements of MACR, NO_x , and the reaction products HCHO, ozone, and different peroxy acyl nitrates (PANs) of several experiments were compared to model results based on the current master chemical mechanism (MCMv3.1). The model runs of the daytime experiments were constrained by measured OH concentrations and measured photolysis frequencies J(O¹D) and J(NO₂).

For the daytime experiments, huge discrepancies between modelled and measured NO_x and peroxyacetylnitrate (PAN) yields could be traced back to shortcomings of the MCM, which deviates from the IUPAC recommendation in some crucial part. By adaption of the recommendation, a much better NO_x , HCHO, and PAN modelmeasurement conformance could be obtained. By comparing the ozone increase during the photolysis experiment, an indirect indication for a model overestimation by a factor of three of the MACR photolysis frequency was found. During nighttime NO_3 chemistry, a yet unexplained overestimation of the methacryloylperoxynitrate (MPAN) yield by both, original MCM and IUPAC adjusted model was observed.