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Mainz Organics Mechanism (MOM): description and sensitivity to some estimated kinetic parameters

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Despite decades of reasearch, global atmospheric chemistry models still have significant biases compared to the estimated distribution and evolution of tropospheric ozone and hydroxyl radical. The gas-phase oxidation of volatile organic compounds (VOC) is acknowledged to play an important role among the processes affecting tropospheric ozone, methane lifetime and aerosol evolution. Thus, chemical mechanisms of very diverse complexity have been developed for the major VOCs. However, all mechanisms present shortcomings such as neglection or lumping of intermediates and estimate of many rate constants and product distributions.

Here, we present a VOC oxidation mechanism of intermediate complexity called the Mainz Organics Mechanism (MOM). With about 400 species and 1500 reactions, it represents the oxidation of about 20 primarily emitted VOCs comprising small alkanes and alkenes, isoprene, pinenes and monocyclic aromatic compounds. The development protocol significantly borrows from the Master Chemical Mechanism (MCM). However, MOM distinguishes itself for a number of features. First, the structure activity relationship for estimating the rate constants involving hydroxyl radical is site-specific and dependent on temperature. Second, the alkyl nitrate yields are considered to be dependent on temperature, pressure and molecular structure. $RO_2 + HO_2$ reaction kinetics is consistent with the recent direct studies of OH-reformation. Isoprene chemistry includes the latest experimental advancements with respect to OH-recycling and alkyl nitrate chemistry. Pinenes chemistry is largely the one by the MCM but with some modifications according to the work of the Leuven's group. Finally, the chemistry of the aromatics is also borrowed from the MCM but with additional photolysis of ortho-nitrophenols leading to HONO formation.

The sensitivity of the model to the temperature and pressure dependence of estimated OH rate constants and alkyl nitrate yields will be investigated and its impact on tropospheric ozone distribution will be shown.