
Abstract

Tropospheric ozone in high concentrations is harmful for mankind and the environment as a whole. As it is a greenhouse gas, its rising due to anthropogenic emissions of the precursor species contributes to global warming. By being the precursor specie for all oxidizing agents in the atmosphere, e.g. the highly reactive OH radical, and being an oxidizing agent itself, ozone is very important in atmospheric chemistry.

Due to this importance, a sound understanding of the chemical ozone production processes is needed. The necessary precursors for the photochemical production are the mainly anthropogenic nitrogen oxides NO_x and the both anthropogenic and biogenic volatile organic compounds. In principle, the processes are fairly understood. In details huge uncertainties still exist. These have to be examined further to allow for well-founded predictions of short and long term ozone concentrations, e.g. to early warn the population off injurious values to come or for the use in climate change modelling.

In the atmosphere simulation chamber SAPHIR chemical processes of the troposphere can be examined nearly without physical caused changes, like transport, mixing, or unknown sources and sinks of trace constituents. Ambient conditions concerning trace gas concentrations, temperature, pressure and lighting conditions characterize the SAPHIR experiments. To understand the complex processes influencing trace gas concentrations in nature, field experiments are obligatory. For the interpretation of measured field data model calculations are needed to distinguish between chemical and physical influences. The test of these models is only feasible under the physically controlled conditions inside the SAPHIR chamber.

In this thesis, three different approaches, which strongly vary concerning their needed (measured) input and the computational effort, for the prediction of the photochemical ozone production were tested against SAPHIR chamber experiments. First of all model runs on the basis of the Master Chemical Mechanism, which compiles the state of the art knowledge in atmospheric chemistry in one mechanism, were tested at ambient trace gas concentrations for the first time. These model runs only need few measured input but a high computational effort. The newly developed First Degradation Step approach in contrast needs a lot of measured input, which then is combined by fundamental arithmetic to calculate the ozone production. The third, also new approach tested is an even simpler method, which estimates the ozone production by a simple combination of measured OH concentrations and OH lifetimes.

As the initial organic compound for the SAPHIR experiments isoprene and its degradation products methacrolein and methyl vinyl ketone were selected,

as on a global scale isoprene is the mostly emitted volatile organic compound, which dominates photochemical ozone production in many regions.

In the second part of this thesis special attention was directed on the methacrolein degradation. The Master Chemical Mechanism model showed strong deviations concerning the measured NO_x concentrations. These discrepancies could partly be explained and were traced back to errors of the Master Chemical Mechanism.