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Evaluation of different SOA schemes using experiments in two outdoor chambers

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Secondary organic aerosols (SOA) constitute a significant fraction of the atmospheric particulate matter. These particles are formed as a consequence of the oxidation reaction of certain organic gases that leads to the formation of low-volatility compounds. Much research has been done during the last years regarding SOA modelling. Since the initial one-step oxidation reaction included in most regional models more complex schemes taking into account the NO_x regime have been proposed. In these schemes the intermediate specie formed from the oxidation of SOA precursors can continue reacting through different pathways depending on the atmospheric chemical conditions. Basically based on chamber experiments, the second-step reaction pathways involve radicals such as HO_2, CH3COO or $CH3O_2$ in low NO_x conditions.

In this study we present an intercomparison of different SOA mechanism (Couvidat et al. 2012, Kim et al. 2011, 1-step scheme currently included in the CHIMERE model) for anthropogenic SOA precursors, and their sensibility to different chemical mechanisms. A comparison of model results against two sets of experiments, performed in two outdoor chambers, EUPHORE (Ceam, Valencia, Spain; Vivanco et al., 2013), and UF (University of Florida, USA) is also included. Experiments in UF were performed for individual VOCs (toluene and 1,3,5 trimethylbenzene), whereas experiments in EUPHORE were focused on a mixture of four anthropogenic VOCs (toluene, 1,3,5 trimethylbenzene, o-xylene and octane).

Regarding the gas phase, a comparison of radical concentration for different chemical mechanisms has been done. Modeled radical concentration was evaluated for one experiment measuring OH and HO_2 concentration.

References:

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