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Modeling the impact of NOx level on secondary organic aerosol formation

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Progressive gas-phase oxidation of volatile organic compounds (VOC) leads to the formation of a myriad of intermediate species. These secondary organic species are more functionalized than their precursor compounds, and the number of functions typically increases as oxidation proceeds. Highly functionalized species have lower vapour pressures and/or higher polarities, allowing substantial partitioning from the gas to the particulate phase, thus leading to the formation of secondary organic aerosols (SOA).

NOx levels control the nature and the distribution of secondary gaseous organics and are therefore suspected to drive SOA yields and speciation. The variation of the SOA yields as a function of NOx levels is difficult to ascertain and remains largely unknown. The objectives of this work are to investigate (i) the influences of tropospheric NOx levels on SOA yields and (ii) how laboratory experiments carried out under high NOx concentrations can be extrapolated to tropospheric NOx conditions.

The sensitivity of the SOA yields to NOx levels will be quantified using a highly detailed model. The model is based on the coupling of explicit schemes for gaseous oxidation with a thermodynamic module. Explicit gas-phase oxidation schemes up to CO2 production were developed using a self-generating approach. The condensation process was parameterised assuming an absorption mechanism.