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Organics chemistry in atmospheric aqueous phase: Development of an explicit modelling tool

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Volatile Organic Compounds (VOC) emitted in the atmosphere are oxidized in complex reaction sequences. This oxidation leads to the formation of secondary VOC which are generally highly soluble and may dissolve into the tropospheric aqueous phase (clouds droplets or deliquescent aerosol). This mass transfer and the subsequent aqueous phase oxidation modify the chemical composition of the aqueous phase as well as the composition of the gas phase after evaporation. Explicit models are useful to characterise the detailed composition of the highly functionalised species and to explore the effects of organics on atmospheric chemistry. The fully explicit representation of hydrocarbon oxidation, from the initial compounds to the final product CO2, requires a very large number of chemical reactions and intermediate species, far in excess of the number that can be reasonably written manually. Such models also require a huge amount of experimental thermodynamic and kinetic data, far in excess of what is currently available in the literature. A self-generating approach, such as the expert system GECKO-A (Generator for Explicit Chemistry and Kinetics of Organics in the Atmosphere), is thus needed to develop fully explicit multiphase oxidation schemes. GECKO-A is currently extended to automatically generate fully explicit oxidation schemes in the aqueous phase on the basis of available kinetic and thermodynamic data and mechanistic studies as well as various estimation methods to evaluate missing information. Preliminary results showing the typical evolutions of secondary VOC in the presence of clouds during the oxidation of terpenes and hydrocarbons will be presented.