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Development and assessement of the GECKO-A multiphase modelling tool for the atmospheric oxidation of biogenic organic compounds

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The evaluation of the impacts of secondary organics on pollution episodes, climate and the tropospheric oxidizing capacity requires modelling tools that track the identity and reactivity of organic carbon in the various stages down to the ultimate oxidation products. 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. We developed a "self generating approach" to explicitly describe (i) the gas phase oxidation schemes of organic compounds under general tropospheric conditions and (ii) the partitioning of secondary organics between gas and condensed phases. This approach was codified in a computer program, GECKO-A (Generator for Explicit Chemistry and Kinetics of Organics in the Atmosphere). This method allows prediction of multiphase mass budget using first principles. However, due to computational limitations, fully explicit chemical schemes can only be generated for species up to C8. We recently implemented a reduction protocol in GECKO-A to allow the generation of oxidation schemes for long chain organics. This protocol was applied to develop highly detailed oxidation schemes for biogenic compounds. The relevance of the generated schemes was assessed using experiments performed in the Caltech smog chamber for various NOx conditions. The first results show a systematic overestimation of the simulated SOA concentrations by GECKO-A. Several hypotheses were tested to find the origin of the discrepancies beetwen model and measurements.