Explicit modeling of the VOC/NOX/SOA system: sensitivity of SOA formation to the gas phase oxidation scheme

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The Generator for Explicit Chemistry and Kinetics of Organics in the Atmosphere (GECKO-A) has been developed to describe highly detailed gas phase oxidation schemes of organic compounds under general tropospheric conditions and the partitioning of secondary organics between gas and condensed phases. This approach leads to the development of chemical schemes involving millions of species and allows the prediction of multiphase mass budgets using first principles. GECKO-A was applied to generate highly detailed oxidation schemes for long chain VOC. The generated schemes for long chain VOC were assessed using smog chamber data for various experimental conditions. Results show a systematic overestimation of the simulated SOA concentrations by GECKO-A. Various sensitivity tests were performed to explore the origin of the discrepancies between model and experimental observations. Results suggest missing gas-phase processes that break the carbon skeleton of the parent compound.