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Development of an explicit model for the formation of secondary organic aerosol

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Volatile organic compounds (VOC) emitted to the atmosphere are oxidized in complex reaction sequences that generate a myriad of intermediates. 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, allowing substantial partitioning from the gas to the particulate phase, thus leading to the formation of secondary organic aerosols (SOA). Understanding SOA formation requires a detailed description of the sources and sinks of species generated during gas phase oxidation. A fully detailed representation of the gradual change of organic compounds leads to the representation of the physical and chemical transformations of a very large number of species, far in excess of the number that can be reasonably managed manually. Data processing tools have to be designed to: (i) describe the detailed evolution of organic compounds in each phase and (ii) provide the relevant physical and chemical properties to parameterise the mass transfer. A model describing explicitly the formation of SOA has been developed. It is based on the coupling of an explicit model for gaseous oxidation schemes with a thermodynamic module. Explicit gas phase oxidation schemes up to CO_2 production were developed using a self-generating approach. The condensation process was parameterised assuming an absorption mechanism. Some preliminary results obtained using this highly detailed scheme are presented.