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Development of a secondary organic aerosols formation mechanism and simulations using a 0-D chemical model

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Formation of secondary organic aerosols (SOA) is a highly uncertain factor in current global chemical models, and consequently is one of the main reasons models cannot properly reproduce aerosol field measurements. A new approach to solve this problem is presented in this work, involving a highly detailed gas-phase chemical mechanism and the condensation of several hydrocarbons the aerosol-phase to produce SOA. Is widely recognized that there are many uncertainties in the mechanism that produces SOA (i.e. the sticking coefficient of semi-volatile compounds on aerosols, enthalpy of vaporization of several compounds, stabilization of the compounds in the aerosol phase due to catalysis); the ultimate goal of this work involves the use of a global 3-D model (IMPACT) to simulate the global production of SOA, including updated emission inventories, a larger number of compounds that can produce aerosols and detailed modeling of the chemical reactions inside the particles.

A module that simulates SOA formation was added to a 0-D model with complete treatment of the chemistry, based on an analysis of odd hydrogen (189 chemical species and 611 chemical reactions). The production mechanism of SOA is through the reaction of selected hydrocarbons with atmospheric oxidants (O_3, OH and NO_3) to produce intermediate first generation products, which are subsequently partitioned between the gas and aerosol phase, over an absorptive medium like primary organic aerosols (mainly insoluble black carbon). The included species with potential to produce SOA are toluene, xylene, aromatic acids and several isoprenes.

The results show the formation of SOA over the time, for different initial conditions and the uncertainty due to uncertain parameters in the formation mechanism.