

Atmospheric evolution of individual organic compounds: an explicit modeling of organic species sources and sinks

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Hundreds of organic species are emitted into the atmosphere. These primary organic compounds (POCs) are mainly hydrocarbons in a gaseous state. They are removed from the atmosphere by reaction with the various tropospheric oxidants (OH, O₃ and NO₃). This atmospheric oxidation involves the formation of thousands of organic intermediates. These secondary organic compounds (SOCs) bear one or more functional groups, such as the alcohol, ketone, aldehyde, hydroperoxyde or nitrates moieties. Some SOCs have a low volatility and/or high solubility in water. They can thus condense on the surface of pre-existing aerosols. These SOCs are removed from the atmosphere by dry deposition (as vapors or particles) or during rain events. The presence of POCs and SOCs in the gas and condensed phases is nowadays known to impact human health, air quality and climate. However, the speciation and the concentration of individual organic species remain largely unknown. Their environmental impact is therefore difficult to quantify.

This study explore the speciation and the evolution of individual POCs and SOCs under various environmental conditions. The sources and sinks of organic compounds are represented explicitly in a box model for various locations and meteorological conditions. Anthropogenic emissions are built using the annual TNO (Netherlands Organization for Applied Scientific Research) inventory⁽¹⁾ coupled to the detailed speciation for non-methane volatile organic compounds provided by Passant⁽²⁾. Biogenic emissions are estimated using emissions potentials provided by MEGAN⁽³⁾ (Model of Emissions of Gases and Aerosol from Nature). Emission of 164 anthropogenic and biogenic organic species are considered in the model. Detailed oxidation chemical schemes for these emitted species are generated using GECKO-A⁽⁴⁾ (Generator for Explicit Chemistry and Kinetics of Organics in the Atmosphere). The chemical schemes includes the formation of 5.4 10⁵ species reacting according to 3 millions of reactions. Deposition is represented in the model using the Wesley⁽⁵⁾ resistance parameterization with effective Henry's law constants estimated for all stable organic compounds using the Grohme⁽⁶⁾ estimation method.

The reliability of the scenarios is evaluated comparing simulated results to NO₂ and O₃ observations available in the Airbase database (<http://acm/eionet.europa.eu/databases/airbase>). The simulations are used here to examine (i) the speciation of major organic species, (ii) their contribution to OH reactivity and nitrogen budget and (iii) their potential transfers towards the condensed phases.

References

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