NCAR | ATMOSPHERIC CHEMISTRY OBSERVATIONS & MODELING

Virtual ACOM Seminar

Kinetics, organic acid yields, and atmospheric impact from the aqueous photooxidation of isoprene-derived organic aerosol compounds

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ABSTRACT

The hydroxyl radical (OH) oxidation of the most abundant atmospheric non-methane hydrocarbon isoprene (C5H8) produces a number of chemical species that partition to the condensed phase via gas-particle partitioning or form condensed-phase compounds via multiphase/heterogeneous chemistry to generate secondary organic aerosols (SOA). The SOA species in aerosol water or cloud/fog droplets may oxidize further via aqueous reaction with OH radicals, among other fates. Regionally, isoprene-derived compounds have been observed as the most abundant individual species in the organic fraction of fine particles, yet, their photochemical fate is not considered in atmospheric models. A gap of information exists for the (1) kinetic rate coefficients, (2) aqueous reaction mechanisms, and (3) yields of key products from of the aqueous photooxidation of isoprene-derived condensed-phased products in chemical systems simulating cloud, fogs and aqueous particles, precluding the atmospheric modeling of the oxidative fate of isoprene-derived SOA. This presentation outlines our recent determinations of (A) the aqueous photochemical kinetic rate coefficients (kOH) for six major isoprene-derived SOA compounds and one analog that were synthesized for study, (B) the aqueous oxidation mechanisms and yields of formic acid (FA) and acetic acid (AA) from isoprene-derived tetrols and organosulfates in the aqueous bulk and particle water; and (C) preliminary GEOS-Chem results on the impacts of this chemistry on both the SOA and FA/AA budgets in the atmosphere. Given that SOA has been overestimated and FA/AA have been underestimated in models over biogenically-rich regions, integrating the aqueous photochemical fate of isoprene-derived compounds (as well as other biogenic SOA species) into models may help resolve both discrepancies.

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