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Exploring the fate of organic molecules in the atmosphere with the hyper-explicit chemical model GECKO-A

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The atmospheric chemistry of organic molecules yields important byproducts (e.g., oxidant gases and organic aerosols) that can harm biota and modify weather and climate. However, this chemical system remains poorly understood because (i) a large number of different organic compounds is emitted by major sources (biogenic, anthropogenic, and pyrogenic hydrocarbons), and (ii) each of these emitted precursors can spawn hundreds of partly-oxidized intermediates differing in their chemical, physical, and optical properties. Only a few of these molecules have been studied directly in the laboratory, so that estimation methods are required for other molecules. We have developed a detailed near-explicit model of hydrocarbon chemistry for the atmosphere, the Generator of Explicit Chemistry and Kinetics for Organics in the Atmosphere (GECKO-A), in which different precursors are oxidized through multiple generations to a myriad of intermediate compounds, and ultimately to CO_2 and H_2O. The model is initialized with available laboratory data where possible, and then uses structure-activity relations (SARs) to estimate kinetics and pathways for reactions lacking direct measurement. This seminar will (i) provide an overview of the organic chemistry relevant in the atmosphere, (ii) give some examples of protocols and SARs used in GECKO-A to extend the applicability of available lab data, (iii) examine model skill in predicting organic particle formation in controlled chamber experiments, and (iv) show some applications to organic budgets on urban, regional, and global scales.

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Refreshments 3:15 p.m.
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