ANALYTICAL SEMINAR

Quantifying Sources and Sinks of Reactive Trace Gases using Chemical Ionization Mass Spectrometry

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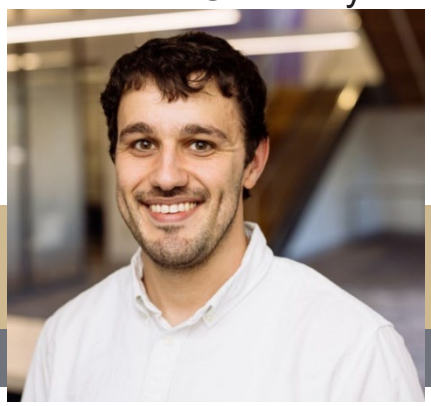

I will present unique mass spectrometry-based methods coupled with micrometeorological techniques used to directly quantify the surface-atmosphere exchange and abundances of volatile organic compounds (VOCs). These surface-atmosphere exchange processes include biogenic and anthropogenic emissions (upward flux) and physical removal via dry deposition (downward flux). Understanding VOC sources and sinks is crucial, as they influence the atmosphere's oxidative capacity and contribute to the formation of particulates and cloud condensation nuclei (CCN), affecting climate both directly by scattering solar radiation and indirectly by altering cloud properties. I will discuss two field studies combining dual high-resolution time of flight chemical ionization mass spectrometers (TOF-CIMS) using H3O+ and I- reagent ion chemistry for comprehensive quantification of VOC mixing ratios and fluxes across two mass spectra. I will then demonstrate how these measurements can be applied to evaluate chemical emissions inventories and atmospheric chemical transport models (CTMs), addressing key scientific questions on VOC sources and sinks, with implications for air quality and climate.

In the first study, we employ the dual TOF-CIMS system to measure VOC fluxes over a pine forest and assess their representation in the state-of-the-art GEOS-Chem CTM. We find that total VOC fluxes are primarily driven by a few key species, including 2-methyl-3-buten-2-ol, monoterpenes, and small oxygenated VOCs, with GEOS-Chem accurately simulating net and upward fluxes. However, far more species contributed to the downward fluxes than are explicitly modeled, leading to a major underestimation of this key sink of atmospheric reactive carbon. In the second study, we use the same TOF-CIMS system to directly quantify VOC emissions over an urban/suburban area on Long Island, NY, during both summer and winter. By applying factor analysis to the data, we identify six key anthropogenic and biogenic emission sectors. We then explore diurnal, weekend/weekday, and seasonal variability to determine the relative importance of local biogenic and anthropogenic VOC emissions, and examine the influence of short-term sources (e.g., personal care products, traffic, cooking) versus persistent sources (e.g., surface evaporation, material decomposition) in shaping overall emissions.

Tuesday, April 1, 2025 | **3:30 pm** | **WTHR 320**

PURDUE UNIVERSITY | James Tarpo Jr. and Margaret Tarpo Department of Chemistry