6.179 New insights into VOC emissions and chemistry using high-resolution chemical-ionization time-of-flight mass spectrometry (H3O+ ToF-CIMS).

Early Career Scientist

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Abstract:

We have recently developed a new chemical-ionization time-of-flight mass spectrometer using H_3O^+ reagent ion chemistry (PTR-MS). The H_3O^+ ToF-CIMS has <1Hz time resolution, with VOC limits-of-detection in the 10s to 100s of ppt's for many atmospherically relevant species. The high mass resolution and time-of-flight operating principle allow simultaneous measurement of more than 1000 VOC ion masses. Here we illustrate significantly improved ability to detect and quantify complex VOC chemistry, using results from recent H_3O^+ ToF-CIMS field deployment, and experimental work with reagent ion chemistry.

The H_3O^+ ToF-CIMS was deployed on the NOAA WP-3 aircraft during the SONGNEX 2015 campaign, targeting emissions from oil and natural gas extraction field in the United States. These regions emit many novel and unexpected hydrocarbon species, and can also be influenced by emissions from urban areas, fires, forests, and agriculture.

Using context from the full mass range measurement, isomerically-specific interpretation of H_3O^+ ToF-CIMS ion masses can be accomplished. Additionally, the high time resolution and many available masses allow the separation of emission sources and chemically distinct air masses within a basin. For example, application of PMF analysis to H_3O^+ ToF-CIMS data from flights over the Denver-Julesburg field in Colorado has enabled the separation of this region's complex, mixed emission sources. Additional field deployment on a mobile laboratory has provided further detailed compositional information.

In further development of this instrument, we have evaluated the use of NO^+ reagent ion chemistry in the ToF-CIMS for measuring VOCs. NO+ CIMS may be an extremely useful technique for measuring aromatics, small aliphatics, semivolatile saturated alkanes, and carbonyl isomers.