

4.013 Synthesizing laboratory and field measurements to trace the bulk oxidation properties and volatility distributions of gas-phase species detected by chemical ionization mass spectrometry.

Early Career Scientist

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Abstract:

We utilize multiple laboratory and field high-resolution time-of-flight chemical ionization mass spectrometry (HR-ToF-CIMS) datasets to assess the volatility distribution and bulk oxidation properties of the identified gas-phase. We find that HR-ToF-CIMS utilizing multiple reagent ions detects species across a large volatility distribution, with species categorized as intermediate-volatility organic compounds (IVOC) dominating the total signal and most influencing the bulk O:C and H:C ratios. We also find that preliminary results in bulk oxidation properties can be extended to differences in aerosol yields of a variety of biogenic volatile organic compounds (BVOCs). Datasets used in this study include small and large chamber experiments of the photo-oxidation of a variety of BVOCs as well as measurement campaigns from sites largely influenced by biogenic sources (southeast US) and a combination of biogenic and anthropogenic source influences (Colorado Front Range). We calculate bulk O:C and H:C ratios for each dataset as a function of oxidant concentrations and ambient conditions. We further determine the volatility distributions of the identified gas-phase species by estimating their vapor pressures based on assumed structure-activity relationships. The calculated vapor pressures were separated into traditional volatility bins, including semi-volatility organic compounds (SVOC), IVOC, and low-volatility organic compounds (LVOC). We determine by signal attribution which volatility bins are most impacting the bulk O:C and H:C values and how the O:C and H:C ratios for each volatility bin change with photo-oxidation and ambient conditions. The bulk oxidation properties of the gas-phase were further extended to aerosol formation and growth in the laboratory and field studies in order to develop a preliminary predictive capability of aerosol yields as a function of the bulk oxidation properties of the precursor gas-phase species.