5.082 Techniques for the ensemble analysis of complex atmospheric mass spectrometric datasets.

Presenting Author:
Jesse Kroll, MIT, jhkroll@mit.edu

Co-Authors:
Abigail Koss, MIT

Abstract:

The last several years have seen an explosion in the amount of data collected by individual atmospheric chemistry instruments. This has been driven in part by the development of new time-of-flight mass spectrometric techniques, which can provide real-time measurements of a large number of different atmospheric organic compounds. While such instruments provide substantial opportunities for gaining new insights into atmospheric composition and chemical processes (from field and laboratory studies), the extreme complexity of the datasets also introduces major challenges in the analysis and interpretation of the measurements. For example it is unclear how such datasets, involving hundreds or thousands of chemical species that each vary with time, can best be used to develop new chemical mechanisms or inform models. Here we investigate the use of advanced analysis approaches for examining such datasets holistically (with species treated together as ensembles rather than individually) for the extraction of useful chemical information. Our focus is on the laboratory (chamber) oxidation of organic compounds, using a number of mass spectrometric instruments to monitor evolving mixtures of reaction products. The datasets (concentrations or intensities as a function of time, from individual instruments or from the combined instrument suite) are analyzed using various ensemble methods (factorization techniques, machine learning approaches, etc.) in order to describe the overall evolving chemistry of the system. A specific objective is to help identify approaches by which results from such laboratory studies can be translated to mechanism or model development.