2.144 Towards comprehensive characterization of atmospheric VOC oxidation products.

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Abstract:

Understanding the oxidation pathways of volatile organic compounds (VOC) in the atmosphere remains challenging for several reasons: the large number of different VOC, the vast amount of different processes they can undergo following reactions with various oxidants, and the perturbation of these processes under varying atmospheric conditions. Nevertheless, new insights are constantly being gained, through both theoretical and experimental efforts. For the latter, recent developments in chemical ionization mass spectrometry (CIMS) have been critical, especially for detecting and quantifying oxidized VOC (OVOC). These OVOC cover a wide range of species, from small volatile fragments (e.g. acetone and formaldehyde) to large highly oxygenated molecules (HOM) able to nucleate and form aerosol particles. No single instrument can map out this entire distribution, yet this is what needs to be done in order to understand OVOC formation processes and their ultimate impacts.

Here, we deployed five different mass spectrometers at our chamber facility to identify to what extent, and under which conditions, there was overlap between the OVOC detected by different instrument types. The system we studied was the oxidation of the monoterpene alpha-pinene, utilizing three CIMS instruments (using nitrate, iodide, and diethylamine as reagent ions) and two proton transfer mass spectrometers (a PTR-TOF and the newly developed VOCUS).

As in earlier studies, we found that two instruments detecting molecules with identical elemental composition is no guarantee for a good correlation between the two. This is also expected, since the selectivity of each instrument is different, and they may thus be measuring different isomers. However, we also found areas of good agreement: the most volatile species were detected by PTR-TOF and VOCUS, semi-volatile species often agreed

between iodide CIMS and VOCUS, and many HOM were identified by both nitrate and amine CIMS. More detailed results and conclusions will be presented during the conference.