# 4.041 Ultra-high Resolution Mass Spectrometric Characterization of Organosulfates in Chinese Aerosols.

Early Career Scientist

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Abstract:

Organosulfates (OSs) are ubiquitous components of particulate matter in atmospheric environment. They are formed as a result of interactions of organic compounds or their oxidation products with acidic sulfate particles. Two types of ultra-high resolution mass spectrometers (UHRMS), Fourier Transform Ion Cyclotron Resonance mass spectrometer (FT-ICR MS) and Orbitrap MS, were used to characterize OSs in aerosol samples collected in the Pearl River Delta, China. With the remarkable resolving power and mass accuracy of UHRMS, hundreds of molecular formulas can be assigned to sulfur-containing compounds (CHOS- and CHONS-), of which OSs possibly make up the majority. FT-ICR and Orbitrap have different mass resolution and mass accuracy. Both have been used to characterize organic aerosols previously, but there isn't comparison of formulas identified by the two UHRMS. In our study employing both UHRMS, 817 OS formulas were identified using FT-ICR while 304 OS formulas using Orbitrap. OS formulas of high *s/n* (>400) detected in FT-ICR analysis was also found in Orbitrap analysis, but for OS formulas of lower s/n, the percentage of overlapping detection by both UHRMS became increasing small with declining *s/n*. The sensitivity difference of the two UHRMS was the dominant cause for accounting for 99% of the discrepancy in the number of identified formulas. Another cause for formula number difference is the superior mass accuracy of FT-ICR (<1ppm) over Orbitrap (<2ppm), as some m/z peaks by Orbitrap could not be assigned a unique formulas and thus not reported previously. This comparison suggests that improved MS analysis optimization with Orbitrap, such as scanning small *m/z* ranges, is needed to minimize mass detection bias. Otherwise part of molecular information would

be lost. The numerous OS formulas identified in this UHRMS study also indicate the high complexity of OS precursors and/or formation pathways in the atmosphere of polluted regions in China.