Relating aerosol mass spectra to composition and nanostructure of soot particles - DTU Orbit (27/09/2019)

**Relating aerosol mass spectra to composition and nanostructure of soot particles**

The composition and carbon nanostructure of soot are important parameters influencing health and climate effects, and the efficacy of soot mitigation technologies. We used laser-vaporization, electron-ionization aerosol mass spectrometry (or SP-AMS) to systematically investigate relationships between aerosol mass spectra, carbon nanostructure (HRTEM), and composition (thermal-optical carbon analysis) for soot with varying physicochemical properties. SP-AMS refractory black carbon concentrations (based on clusters) were correlated to elemental carbon ($r=0.98$, $p<10^{-8}$) and equivalent black carbon (aethalometer) concentrations. The SP-AMS large carbon ($C^+≥6$, midcarbons and fullerene carbons) fraction was inversely correlated to fringe length ($r=-0.97$, $p=0.028$) and linearly correlated to the fraction of refractory organic carbon that partially pyrolyze during heating ($r=0.89$, $p<10^{-4}$). This refractory organic carbon material was incompletely detected with conventional aerosol mass spectrometry (flash vaporization at 600°C). This suggests that (SP-AMS) refractory carbon cluster analysis provides insight to chemical bonding and nanostructures in refractory carbon materials, lowcarbons ($C^+≥5$) indicate mature soot and large carbons indicate refractory organic carbon and amorphous nanostructures related to $C_5$-components. These results have implications for assessments of soot particle mixing state and brown carbon absorption in the atmosphere and enable novel, on-line analysis of engineered carbon nanomaterials and soot characteristics relevant for climate and health.

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