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Apportionment of Size Distribution Data from the Aerodyne Aerosol Mass Spectrometer in Pittsburgh and Mexico City

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Aerodyne aerosol mass spectrometers (AMS) collect spectra of ambient aerosols that are a mix of various primary and secondary sources. Many recent studies have reported the identification of sources / components based on factor analysis of total mass spectrum mode (bulk submicron) data (e.g. Zhang et al., ES&T 2005; ACP 2005; GRL 2007; Lanz et al., ACP 2007; Ulbrich et al., ACP 2009; Aiken et al., ACP 2009; Huffman et al., ACP 2009; Slowik et al., ACPD 2009). Data collected in the PToF (particle time-of-flight) mode of the AMS represent chemical composition as a function of particle size (vacuum aerodynamic diameter). We conceptualize these data as a 3-dimensional matrix and discuss the various approaches to their factorization in order to investigate the information content about aerosol sources and processing. Factoring the size distribution data utilizes an additional dimension of information that may allow greater factor separation than using the mass spectral mode data alone. We briefly review previous applications of factor analysis to size distribution data (chemically resolved and not). We use the Multilinear Engine (Paatero, J. Comput. Graph. Stat., 1999) to determine the changing size distribution and concentration of chemical components (e.g., sulphate, nitrate, and types of organic aerosol (OA) including oxidized (OOA), hydrocarbon-like (HOA), and biomass-burning (BBOA)). We demonstrate the method with AMS datasets acquired in Pittsburgh in 2002 (Q-AMS; Zhang et al., ES&T 2005; Ulbrich et al., ACP 2009) and Mexico City in 2006 (HR-ToF-AMS; Aiken et al., ACP 2009). To our knowledge this is the first attempt to factorize highly time- and size-resolved composition data.