



Chemometric analysis of multi-sensor hyperspectral images of coarse mode aerosol particles for the image-based investigation on aerosol particles

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Multi-sensor hyperspectral imaging is a novel technique, which allows the determination of composition, chemical structure and pure components of laterally resolved samples by chemometric analysis of different hyperspectral datasets. These hyperspectral datasets are obtained by different imaging methods, analysing the same sample spot and superimposing the hyperspectral data to create a single multi-sensor dataset.

Within this study, scanning electron microscopy (SEM), Raman and energy-dispersive X-ray spectroscopy (EDX) images were obtained from size-segregated aerosol particles, sampled above Western Australian salt lakes. The particles were collected on aluminum foils inside a 2350 L Teflon chamber using a Sioutas impactor, sampling aerosol particles of sizes between 250 nm and 10 μm . The complex composition of the coarse-mode particles can be linked to primary emissions of inorganic species as well as to oxidized volatile organic carbon (VOC) emissions. The oxidation products of VOC emissions are supposed to form an ultra-fine nucleation mode, which was observed during several field campaigns between 2006 and 2013.

The aluminum foils were analysed using chemical imaging and electron microscopy. A Horiba LabRam 800HR Raman microscope was used for vibrational mapping of an area of about 100 μm x 100 μm of the foils at a resolution of about 1 μm . The same area was analysed using a Quanta FEI 200 electron microscope (about 250 nm resolution). In addition to the high-resolution image, the elemental composition could be investigated using energy-dispersive X-ray spectroscopy. The obtained hyperspectral images were combined into a multi-sensor dataset using the software package Imagelab (Epina Software Labs, www.imagelab.at). After pre-processing of the images, the multi-sensor hyperspectral dataset was analysed using several chemometric methods such as principal component analysis (PCA), hierarchical cluster analysis (HCA) and other multivariate methods. Vertex component analysis (VCA) allowed the extraction of single spectra of pure components such as gypsum, NaNO_3 and oxidized VOC).

Different aerosol species related to the salt lakes (e.g. inorganic salts) and the surrounding land (e.g. silica particles) could be uncovered. Furthermore, the interaction of primary particles with volatile organic species, released from remains of the former eucalyptus forests and crop plants, could be identified. The application of multi-sensor imaging to size-segregated laterally resolved aerosol particles deepens the understanding of composition, linkage, interfaces and single components of complex mixtures of atmospheric aerosol particles, and therefore gives access to an intrinsic understanding of the nature of these particles.