Coagulation versus chemical processing in a single particle mass spectral data set

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Single particle aerosol mass spectrometers, like the LAAPTOF (Laser Ablation Aerosol Particles Time of Flight mass spectrometer) produce large amounts of data. For each individual particle, a bipolar mass spectrum and the vacuum aerodynamic diameter are recorded. To efficiently analyze these data sets, it is important to use visualization techniques which highlight the important features of the data.

Recently, we successfully combined the classical c-means cluster algorithm (Bezdek, 1981) with the OPTICS algorithm (Ankerst *et al.* 1999). The key feature of the combination of these algorithms is their ability to visualize continuous variation of the composition of particles in an aerosol (Reitz *et al.* 2016, submitted). This first application of the OPTICS algorithm in the field of aerosol science was based solely on the mass spectra. Adding the size of the particles to the visualization, we are able to visualize the coagulation of two particle populations within the aerosol.

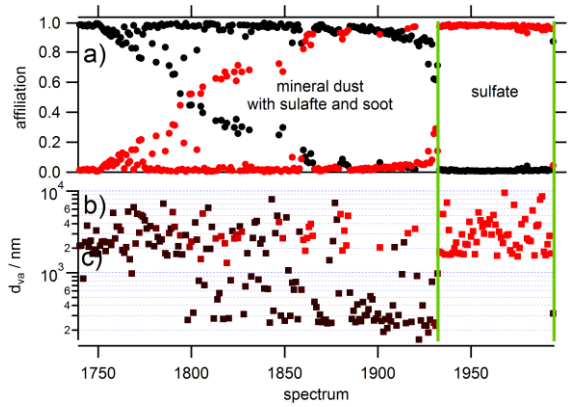

Figure 1. Visualization of coagulation within an aerosol population. a) Affiliation to the two relevant fuzzy c-means classes. b) Particle size: The color code indicates the affiliation to the red class.

Figure 1 shows an extract of the dataset for which coagulation has been visualized. The data has been ordered using the OPTICS algorithm. The left part of the graph contains particles which have been attributed to a mixture of mineral dust, soot and sulfate. The right part of the graph shows mainly signatures of sulfate salts in the mass spectra. Figure 1a displays the affiliation of the particles to the two relevant c-means classes (black class and red class). In the left region, most particles are affiliated to the black class. However, from left to right, the affiliation to the red class continuously grows for some particles. In the right region, the red class receives close to 100 % of the affiliation.

In Figure 1b, we present the size of the particles, colored by the degree of affiliation to the red class. The black class is composed of two size modes, one peaking around 2 µm and one peaking around 300 nm. In contrast the red class is solely composed of large particles with sizes around 2 µm. In our presentation we will show how to identify physical coagulation of particles and distinguish it from chemical processing.

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