Cite abstract as Author(s) (2009), Title, European Aerosol Conference 2009, Karlsruhe, Abstract T024A01

Cluster analysis on mass spectra of biogenic secondary organic aerosol

C. Spindler[1], A. Kiendler-Scharr[1], E. Kleist[2], A. Mensah[1], Th. F. Mentel[1], R. Tillmann[1] and J. Wildt[2]

[1] Institut für Chemie und Dynamik der Geosphäre, ICG-2, Forschungszentrum Jülich, Germany
[2] Institut für Chemie und Dynamik der Geosphäre, ICG-3, Forschungszentrum Jülich, Germany

Keywords: Statistical analysis, Aerosol mass spectrometry, SOA, Biogenic Particles

Biogenic secondary organic aerosols (BSOA) are of high importance in the atmosphere. The formation of BSOA from the volatile organic compound (VOC) emissions of selected trees was investigated in the JPAC (Jülich Plant Aerosol Chamber) facility (Mentel et. al., 2009). The tree emissions mainly consist of monoterpenes, sesquiterpenes and organic VOC. The gases were transferred into a reaction chamber and BSOA was formed by OH and O_3 oxidation. The chemical composition of the aerosol was characterized by aerosol mass spectrometry (Aerodyne Quadrupol-AMS, Jayne et. al., 2000). Inside the AMS, the aerosol particles are flash-vaporized at 600°C and the evaporated molecules undergo electron impact ionization at 70 eV. These processes cause a high fragmentation of the organic compounds which is reflected in complex mass spectrometric patterns.

Here, we present a classification of the aerosol mass spectra via cluster analysis (Marcolli et. al., 2006). This method computes a mathematically defined distance between all pairs of mass spectra in a dataset (Figure 1). Similar mass spectra have smaller distances than unlike mass spectra. Average mass spectra are produced by combination of single mass spectra to so-called clusters. The clustering starts with the two closest mass spectra and progresses with increasing distance. This process is visualized with a dendrogramm (Figure 2), where the single clustering steps can be retraced.

The mass spectra presented here were similar compared to ambient mass spectra due to the similarity of the precursor substances. However, we can show that there are differences in the BSOA mass spectra of different tree species. Furthermore we can distinguish the influence of the precursor chemistry and chemical aging. BSOA formed from plants exposed to stress can be distinguished from BSOA formed under non stressed conditions. Significance and limitations of the clustering method for very similar mass spectra will be demonstrated and discussed.

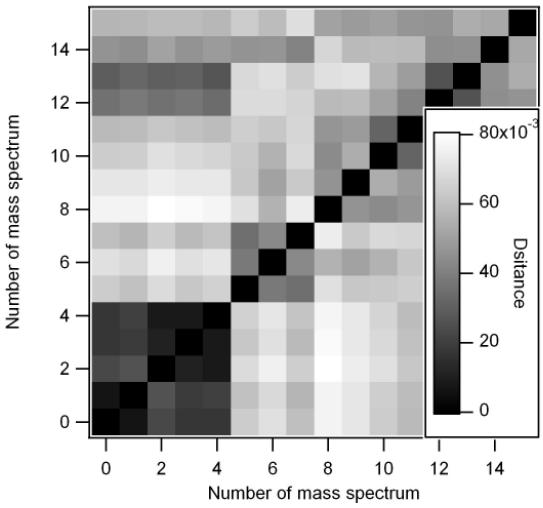

Figure 1. Pairwise distance of mass spectra

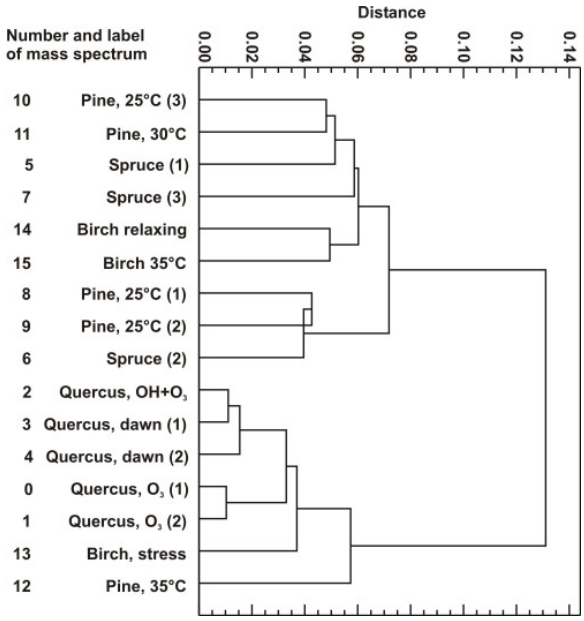

Figure 2. Dendrogramm of cluster analysis

Jayne, J. T., et. al. (2000). *Aerosol Science and Technology*, 33, 49-70.

Marcolli, C., et. al. (2006). *Atmospheric Chemistry and Physics*, 6, 5649-5666.

Mentel, Th. F., et. al. (2009). *Atmospheric Chemistry and Physics Discussions*, 9, 3041-3094.