

Comprehensive analysis of anthropogenic aerosol using automated classification for GCxGC-TOF analysis

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The Virtual Helmholtz Institute (HICE) addresses the health effects of anthropogenic combustion processes. This is performed by means of a joint comprehensive characterization of the chemical and physical properties of the investigated combustion aerosol as well as the biological effects on cell cultures with high-end innovative methods. With targeted analyses based on chromatography and mass spectrometry a wide range of important analytes could be quantified. (Lintelmann, 2010; Orasche, 2011) However, the complexity of combustion aerosols exceeds the capacities of such targeted methods and instrumentation by far. Comprehensive two dimensional gas Chromatography is a very promising tool to extend the number of accessible analytes even further.

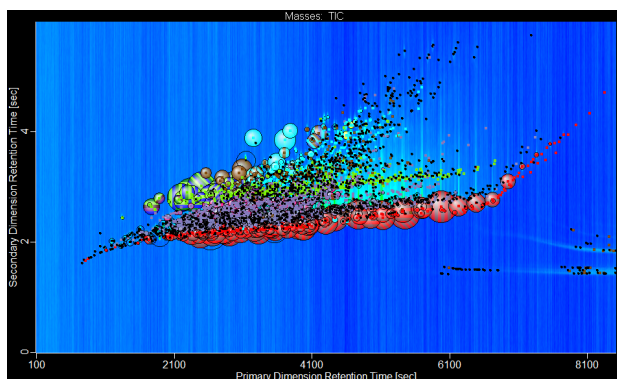


Figure 1: Bubble plot of an urban aerosol sample obtained after using the developed scripting. The different colors indicate several substance classes.

Comprehensive two-dimensional gas chromatography time-of-flight mass spectrometry: Automated Classification and Non-targeted automated comparison of semi-volatile organic compounds

Multidimensional Gas-Chromatography is well suited for the comprehensive characterization of complex sample compositions. However, the huge amount of data reveals also some drawback of the technique. This is the difficult and troublesome evaluation of the obtained data. Not at least because of this disadvantage the multidimensional gas-chromatography is little used in the field of aerosol science (Welthagen, 2003).

Nevertheless, aerosols represent complex mixtures of substances and therefore GCxGC should be most suited for analyzing. The first approach focuses on a semi-quantitative comparison of substance classes. Current attempts for an automated classification of substance classes are being made in order to simplify the data evaluation. Most commercial available data processing software, e.g. from LECO, had embedded features to use customized algorithms for classification (Vogt, 2007; Welthagen, 2005). These classification algorithms are based on knowledge based rules. Within the scope of the HICE project advanced scripting rules for the comprehensive analysis of semi volatile organic compounds were developed and applied to compare the chemical composition of particulate matter from different combustion sources.

The enhanced separation power of GCxGC combined with state-of-the-art deconvolution technologies offers also the opportunity to align and compare thousands of jet not identified peaks semi-quantitatively on a molecular level.

References

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