ME-2 analysis of long-term on-line mass spectrometric data of non-refractory submicron aerosol in the city of Zurich

F. Canonaco\textsuperscript{a}, J. G. Slowik\textsuperscript{a}, U. Baltensperger\textsuperscript{a}, A.S.H. Prévôt\textsuperscript{a}

\textsuperscript{a}Laboratory of Atmospheric Chemistry, Paul Scherrer Institut, 5232 Villigen PSI, Switzerland

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Presenting author email: francesco.canonaco@psi.ch

The role of aerosols in the atmosphere is of importance, because they affect climate (Forster et al., 2007), human health (Peng et al., 2005), ecosystems, e.g., acidification (Matson et al., 2002), and visibility (Watson, 2002). Thus, the identification and quantification of formation mechanisms and sources is of high priority. However, this task is complicated due to the complexity of particle composition.

Long-term monitoring of aerosol composition provides a powerful tool for the analysis of the aforementioned effects. Long-term measurements allow capturing the seasonal variability of different aerosol constituents, which is not possible with shorter-term campaigns. Furthermore, long-range, mesoscale, and local air quality models can be improved through comparison with long-term datasets. Finally, the existence of long-term sampling records at a given site provides a framework for the interpretation of datasets from short-term intensive measurement campaigns.

We present measurements of submicron aerosol composition from an aerosol chemical speciation monitor (ACSM, Aerodyne Research, Inc.) deployed in downtown Zurich. The ACSM yields quantitative mass spectra of the non-refractory aerosol component with an averaging period of 15 to 30 minutes. These are one of the first full-year measurements in Europe using this technique. As shown in Fig. 1, the ACSM is capable of resolving inorganic species such as NH\(_4\), SO\(_4\), NO\(_3\), Cl, and the organics. The data can be further deconvolved in order to identify and apportion the sources, in particular for the complex organic fraction.

There are several possible techniques for the deconvolution of a data set. Positive matrix factorization (PMF) has been extensively exploited for this type of data. However, the multilinear engine 2 (ME2) offers advantages compared to PMF, due to the fact that the user has the possibility to introduce a priori information in form of e.g. known factor profiles into the model (Paatero, 1999).

The aim of this work is to make use of the multiple approaches available in ME2 on a large dataset, in particular on the obtained data from downtown Zurich during the full year 2011. For this purpose we implemented a user-friendly interface in the software IGOR Pro (Wavemetrics, Inc.) which shall be shared in the next future with other research groups.

We will discuss identification and source apportionment of ACSM organic data at an urban site over the full year of 2011 with the ME-2 algorithm. Different techniques, like the a-value (Lanz et al., 2008) or the pulling approach (Paatero, P. and Hopke, P.K., 2009), as highlighted in Fig.2 have been tested. Moreover, studying and comparing the outcomes of these just mentioned techniques provides useful information for estimating of the model uncertainty.

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