



Source contributions of semi volatile organic compounds in ambient PM_{2.5}

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Organic compounds have been used as source indicators for source apportionment in aerosol research for many years [1]. In our investigation, concentrations of low volatile organic compounds measured in Augsburg, Germany are analysed using positive matrix factorisation (PMF) [3], to identify sources and to estimate source contributions. PM_{2.5} ambient urban air particulate matter was at an inner city sampling site in Augsburg, Germany. 24 h low-volume samples (1 m³ h⁻¹) were samples from January 2003 through December 2004. Chemical analysis of SVOC in the PM_{2.5} samples was done by direct thermal desorption-gas chromatography-time of flight mass spectrometry, DTD-GC-TOFMS. Analysis was done for about 200 compounds. 78 compounds on 620 days were used for PMF analysis. Solutions with 5 factors turned out to be the most plausible and interpretable ones amongst all calculated solutions. All compounds exhibited distinct seasonal variations in concentration. Most compounds had highest concentrations during the cold seasons with a distinct, source depended pattern. E.g. the homohopane index could be used to separate between coal and mineral oil derived emission. Dehydro abietic acid methyl ester (DHAM) for instance indicated wood burning emissions in Winter. In summer, e. g. long chain n-alkanones and 6,10,14-trimethylpentadecanone (a oxidation product of chlorophyll) had the highest concentrations. Using positive matrix factorization (PMF) for the statistical investigation of the data set five factors have been separated. These factors are dominated by the pattern of single sources or groups of similar sources, factor 1 - lubricating oil, factor 2 - emissions of diesel and heating oil consumption, factor 3 - Wood combustion, factor 4

- brown coal combustion and factor 5 - biogenic emissions and transport components. Like the SVOC the factors showed strong seasonality with highest values in winter for factor 1 to 4 and in summer for factor 5. It was evident, that no factor could be separated which defines exclusively a single source. However, all five factors are clearly dominated by a single source or a group of similar sources. In the presence of two or more factors with very similar variation in time (as for instance domestic heating with different fuels in the cold season) statistical approaches like PMF may have difficulty in the separation of these sources in the time series analysis.. The assumption of a constant pattern of the factors, independent of emission conditions, may contribute to this fuzziness, too.

Keywords: Semi volatile organic compounds (SVOC), Positive Matrix Factorisation (PMF), Source apportionment

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