Chemical investigation of eight different types of carbonaceous particles using thermoanalytical techniques

G. Matuschek1, E. Karg2, A. Schröppel2, H. Schulz2, O. Schmid2

1GSF-National Research Center for Environment and Health, GmbH, Institute of Ecological Chemistry, Ingolstädter Landstraße 1, D-85764 Neuherberg, Germany
2GSF - National Research Center for Environment and Health, GmbH, Institute of Inhalation Biology, Ingolstädter Landstraße 1, D-85764 Neuherberg.

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The chemical composition of ambient aerosol particles affects numerous important physical aerosol parameters as well as their potentially adverse health effects. In recent years, numerous epidemiological studies have revealed an association between elevated levels of ambient particles and increases in all-cause morbidity or mortality. Recently, toxicological and epidemiological studies indicate that ultrafine particles (< 0.1 µm diameter) may be more harmful per unit mass than larger ones (Oberdörster 2000).

However, the studies suffer from a lack of detailed information on particle chemistry. Some newer studies (Stoeger et. al 2006, Schober et. al. 2006) try to overcome this limitation. These and other studies have characterized carbonaceous particles based on the thermooptically determined organic carbon (OC), elemental carbon (EC) content and the ratio of both. Unfortunately, the interpretation of the resulting OC/EC data is limited by the fact that, OC and EC are operationally defined parameters, i.e., the observed OC and EC content is method-dependent (Chow et. al. 2001). In addition, the methods can not provide detailed chemical speciation, a drawback that is particularly significant for toxicological or biological studies, and the organic matter content needs to be calculated from OC by conversion factors.

The objective of this study was to derive both detailed chemical speciation and useful proxies for the quantitative classification of the organic matter content of carbonaceous aerosol samples. Using three different techniques, a) thermal desorption - gas chromatography mass spectrometry (TD-GC/MS), b) evolved gas analysis with mass spectrometry (EGA-MS) and c) thermogravimetry with Fourier transform infrared spectroscopy (TG-FTIR), we investigated eight different carbonaceous particulate matter samples used for health effect studies. The samples include different types of surrogate soot particles, pigment black and spark-generated carbon particle as well as two ambient aerosol samples (diesel soot and particulates collected in a road tunnel). All samples showed an increasing mass desorption (Md) with rising temperature, but the desorption curves scattered heterogeneously allowing no reliable OC classification based Md alone. However, as seen from Fig. 1, the samples could be clearly distinguished based on their OC content (high/low OC samples = solid/open symbols) using a novel parameter, the "equivalent organic mass fraction" OMF, where OMF = OIR*Md ("organic ion ratio" OIR is the ratio of the areas underneath the “organic” and total ion count signal of the EGA-MS).

![Figure 1. OIR versus Md. The contour lines represent the 5%, 10% and 15% levels of the OMF]({{endpoint}}/images/chemical_investigation.png)

The validity of this classification was confirmed with a second proxy parameter and information on the generation process of the particles. Both types of printex samples and the spark-generated carbon particles showed the lowest OC mass fraction (<8%), whereas for road tunnel and diesel emission particles <16 % and <19 % was estimated, respectively.