Estimation of Organic and Elemental Carbon using FT-IR absorbance spectra from PTFE Filters

M. Reggente[1], A. M. Dillner[2] and S. Takahama[1]

[1] Atmospheric Particle Research Laboratory, EPFL, Lausanne, Switzerland
[2]University of California, Davis, Davis, California, USA
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Presenting author email: matteo.reggente@epfl.ch

Organic carbon (OC) and elemental carbon (EC) are the major components of atmospheric particulate matter (PM), which has been associated with increased morbidity and mortality, climate change and reduced visibility. Typically OC and EC concentrations are measured using thermal methods such as thermal-optical reflectance (TOR, Chow et al., 2007) from samples collected on quartz filters. However, TOR measurements are destructive and relatively expensive.

Methods

Here, we present an extension of the work of Dillner and Takahama (2015a) and Dillner and Takahama (2015b). We have used the FT-IR absorbance spectra and TOR OC and EC concentrations collected in the Interagency Monitoring of PROtected Visual Environment (IMPROVE) network (USA). We used 517 samples collected in 2011 in seven sites to calibrate the models, and more than 2000 samples collected in 2013 at 17 sites – samples from six sites are present both in the calibration and test sets – to test the models.

We estimate OC and EC using Fourier transform infrared (FT-IR) from Teflon (PTFE) filters using partial least square regression (PLSR). The proposed method can reduce the operating costs of large air quality monitoring networks: the analysis technique is inexpensive, non-destructive and fast. It uses routinely collected PTFE filter samples that, in addition to OC and EC concentrations, can concurrently provide information regarding the composition of organic aerosol (Ruthenburg et al., 2014; Takahama et al. 2013).

Results

Figure 1 shows the estimations of the OC and EC concentrations for the year 2013 of the samples collected in the same six sites present in the calibration set (year 2011). The models produce precise and accurate estimations ($R^2 \geq 0.93$).

We will also show results and discuss the quality of estimations (for the year 2013) of samples collected at the remaining 11 sites not included in the calibration set. In the discussion, we will also propose a statistical modelling technique to anticipate the estimation error and give confidence in the goodness of the estimation. We will show how to discriminate between not reliable estimations – samples that are not accurately modelled with the available calibration dataset – and reliable estimations.

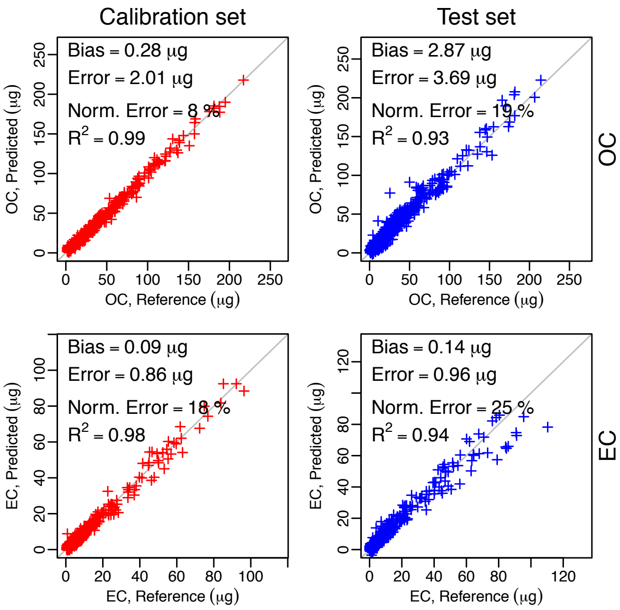

Figure 1. Model results: Predicted FT-IR OC and EC versus measured TOR OC and EC.

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Chow, J.C., Watson, J.G., Chen, L.W. A., Chang, M.C. O., Robinson, N.F., Trimble, D., and Kohl, S. (2007) *J. Air Waste Manage.*, 57, 1014–1023, 2007.

Dillner, A.M. and Takahama, S. (2015a) *Atmos. Meas. Tech.,* 8, 1097–1109.

Dillner, A.M. and Takahama, S. (2015b) *submitted to Atmos. Meas. Tech. Disc.*

Ruthenburg, T.C Perlin, P.C., Liu, V., McDade, C.E., and Dillner, A.M. (2014) *Atmos. Environ.,* 86, 47–57.

Takahama, S., Johnson, A., and Russell, L. M. (2013) *Aerosol Sci. Technol.,* 47, 310–325.