Determination of Organic Material to Organic Carbon (OM/OC) Ratios by FT-IR Spectroscopy at Select Sites in the IMPROVE Network

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Organic carbon (OC) in $PM_{2.5}$ (particulate matter (PM) with an aerodynamic diameter $\leq$2.5 μm) filter samples is typically quantified using a thermal optical technique for samples collected on quartz filters. After correcting the OC mass for gas phase adsorption, mass of organic matter (OM) in $PM_{2.5}$ is estimated by multiplying OC by a fixed factor that typically ranges from 1.4 to 1.8. In this work, we develop a non-destructive, Fourier Transform-Infrared spectroscopic (FT-IR) technique to measure OM in $PM_{2.5}$ samples collected on PTFE filters (polytetrafluoroethylene, commonly called "teflon filters"). PTFE filters are used for gravimetric, light absorption and elemental analysis in the IMPROVE network and the non-destructive FT-IR technique does not interfere with those analyses. Gas phase adsorption onto PTFE filters is negligible so no sampling artifact correction is needed. FT-IR measures absorption by organic functional groups, which are comprised of carbon bonded to oxygen, hydrogen and other elements. To calibrate the method, we developed laboratory standards of atmospherically relevant organic compounds collected on PTFE filters and measured their absorption using a standard FT-IR instrument. A multivariate calibration based on the laboratory standards was used to quantify organic functional groups, including alkane CH, alcohol OH, carboxylic acid OH, and carbonyl. These four functional groups are likely to represent the preponderance of organic mass in most ambient aerosol samples. OM is estimated using a weighted sum of all functional groups and OC is estimated using a weighted sum of the alkane CH and carbonyl functional groups. The precision of the OM measurement is 7% and the minimum detection limit is 0.15 $\mu g/m^3$ for an IMPROVE sample.

The method was employed to estimate OM, OC, OM/OC and organic functional groups in one year of routinely collected filter samples at seven IMPROVE sites. In the IMPROVE network protocol, OC is measured using a thermal optical reflectance method and OM is estimated using an OM/OC ratio of 1.8. Using the FT-IR technique developed here, the median OM/OC ratio for the seven sites was 1.67 and the 25^{th} and 75^{th} percentiles were 1.53 and 1.86. Phoenix, AZ had the lowest median value of 1.55 and Mesa Verde, CO had the highest of 1.83. For most sites, the highest median OM/OC ratio occurred in fall while the lowest occurred in winter or spring. The FT-IR measured sample, site and seasonal OM/OC ratios indicate that a single estimate of OM/OC does not represent the observed variability in OM/OC. Additionally, the mass of functional groups vary by sample, site and season.

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