

Development of a non-destructive method based on infrared analysis for quantification of ionic components in atmospheric particulate matter

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Among the analytical techniques developed so far for atmospheric aerosol characterization, Fourier Transform Infrared spectroscopy (FTIR) allows to determine both organic fraction (functional groups) and some inorganic components (ammonium, nitrate, sulfate, silicates, carbonates). The FTIR analysis on particulate matter collected on filters has encountered great success since the method is basically not destructive so that the sample can be analyzed further using other techniques. It is worthy to note that the approaches used in the literature to determine the above mentioned aerosol components generally involve rinsing the sample with appropriate solvents (Maria et al., 2002; Russel et al., 2009).

In this work we focus on the quantification of the inorganic components of PM (NO_3^- , SO_4^{2-} , NH_4^+) by FTIR and therefore avoiding any sample pre-treatment. Of each sample was recorded in the absorption spectrum transmittance. To obtain quantitative information from the FTIR spectra, a multivariate approach based on Partial Least Squares (PLS) has been applied.

The samples themselves were used as standards for the training of the multivariate model; input data were obtained analyzing the samples with ion chromatography (Piazzalunga et al., 2013).

The development of PLS models was performed on a database of 300 filters collected in several measurement campaigns carried out in Milan and Genoa between 2010 and 2012.

A preliminary analysis of IC data with Principal Component Analysis (PCA) shows how the first two principal components explain 98% of the total variance. Five different PLS models were tested. The number of latent variables for each model was chosen minimizing RMSECV (error in cross validation).

The models for the examined species show a good agreement with IC data, in figure 2 is reported the comparison between FTIR and IC sulphate quantification.

In conclusion, coupling FTIR with PLS methods allows to quantify major ions in PM samples without pre-treatment reducing costs and time of analysis.

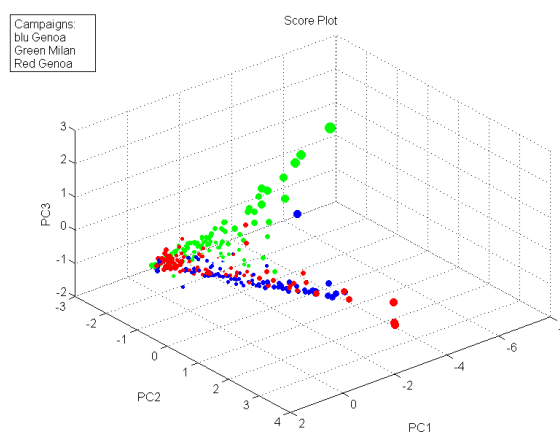


Figure 1: score plot obtained from PM compositional data (sulphate, nitrate and ammonium); variance explained by PC1 and PC2: 98%

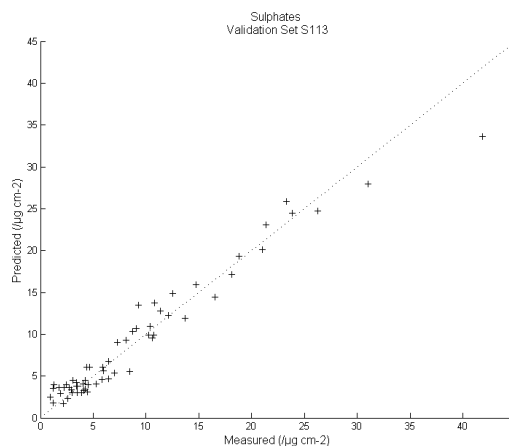


Figure 2: Comparison between FT-IR (y axis) and ion chromatography (x axis) sulphate quantification

References

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- Russell et al., 2009, *Atmospheric Environment*, 43(38), 6100-6105
- Maria et al., 2002, *Atmospheric Environment*, 36(33), 5185-5196