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Non-destructive method based on infrared spectroscopy and partial least square regression for the quantification of the ionic component of atmospheric particulate matter

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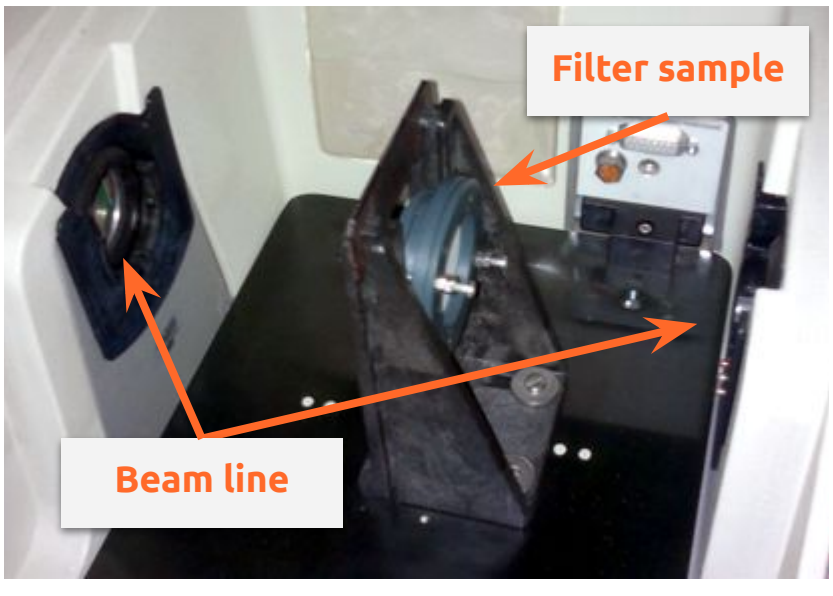
Motivation Atmospheric aerosols influence radiative forcing and have a negative impact on air quality especially in urban scenarios. The adverse impact on urban air quality is a prominent societal and health issue, expected to become more and more severe in the future. In order to introduce effective mitigation strategies and monitor their effect, the state and characteristics of pollution need to be characterized and main sources identified. Offline-analysis offers such insight. However, PM chemical composition is highly complex, and its comprehensive characterization and quantification requires advanced instrumentation and data analysis techniques and strategies.

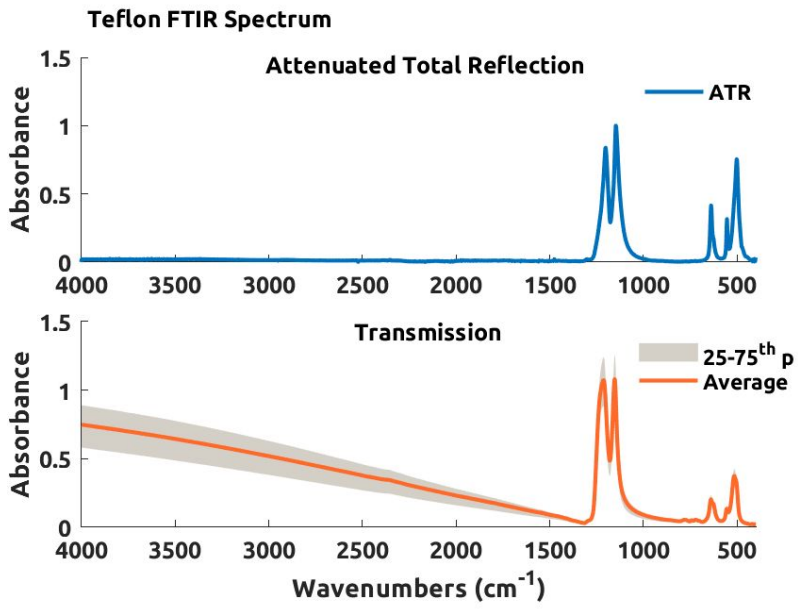
Sample collection We acquired Fourier-transform infrared spectroscopy (FTIR) spectra of ambient PM collected on Teflon filters at various locations in Italy. FTIR allows to obtain high-resolution spectral data non-destructively and therefore to detect and quantify functional groups of organic and inorganic species present in the aerosol PM.

Dataset		
Campaign (filter n°)	**Filter**	**PM**
I (84)	Teflon	2.5
II (113)	Teflon + Quartz	1
III (39)	Teflon	10
IV (55)	Teflon + Quartz	2.5

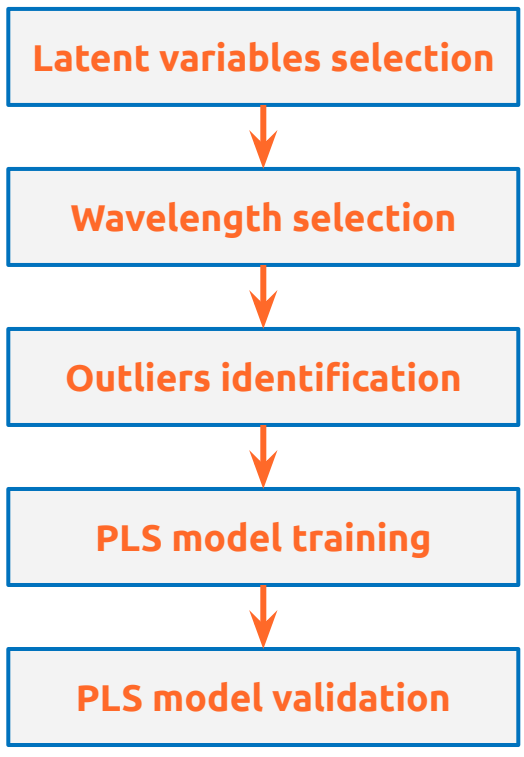
Sample analysis Filter samples are placed on a 3D printed holder and spectra are recorded in transmission. (range: 400-4000 cm^{-1}, resolution: 4 cm^{-1}, 128 scans). Ion chromatography analysis provides the concentration for ammonium, nitrate and sulfate PM component



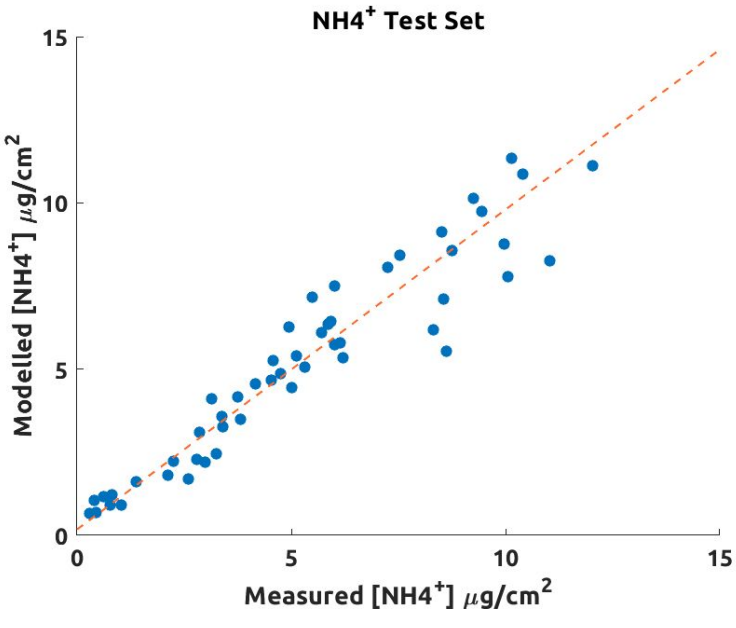
Teflon FTIR study



PLS workflow



Results



Conclusion PLS regression methods, applied to FTIR spectra of PM teflon filters, allowed us to develop a robust, low cost and non destructive analytical method for the quantification of ammonium, nitrate and sulfate in PM samples. This method can also be extended to other chemical components.

References

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