An Automated Baseline Correction Method for Atmospheric Aerosol Infrared Spectra Collected on Polytetrafluoroethylene (Teflon) Filters

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Keywords: Teflon, baseline correction, FT-IR
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A growing volume of research on statistical applications for characterization of atmospheric aerosol Fourier Transform Infrared (FT-IR) samples collected on polytetrafluoroethylene (PTFE) filters (e.g., Russell et al., 2011) and a rising interest in analyzing FT-IR samples collected by air quality monitoring networks highlight the need for an automated PTFE baseline correction method. The existing polynomial technique (Takahama et al., 2013) remains unscalable to projects with a large amount of aerosol samples because it requires expert intervention in fine tuning several parameters.

Therefore, the question of how to develop an automated method for baseline correcting hundreds to thousands of atmospheric aerosol spectra given the variability in their aerosol mixture composition remains. We address the question by introducing the statistical protocol, which allows for the precise definition of analyte and background sub-regions, applies non-parametric smoothing splines to reproduce sample-specific PTFE variations, and integrates performance metrics from atmospheric aerosol and blank samples alike in the smoothing parameter selection.

Referencing an extensive set of atmospheric aerosol samples from several Interagency Monitoring of PROtected Visual Environment sites, we identify key FT-IR signal characteristics (such as non-negative absorbance or analyte segment transformation), which reduce signal variations to fundamental features to capture sample-specific transitions between background and analyte. To reproduce unique variations in PTFE background and analyte structures, we apply an adaptive interpolation based on smoothing splines modulated by the sample-specific roughness parameter.

One of the applications for characterization of ambient aerosol FT-IR samples include unsupervised clustering of discrete spectra categories to quantify source contributions, such as fossil fuels or biomass burning, to the total organic mass. Another approach with a long record in use for quantification of functional group composition and source apportionment is fitting individual Gaussian lineshapes to quantify alcohol COH, carboxylic COH, alkane CH, carbonyl CO, and amine NH functional groups (Takahama et al., 2013). An example of an uncorrected (raw) spectrum and baseline corrected spectrum with fitted functional groups is shown in Fig 1.

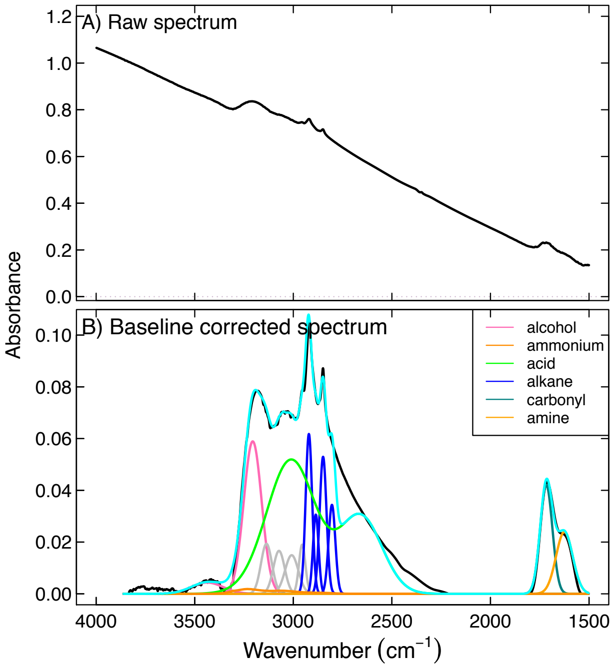

Fig 1: A) Raw and B) baseline corrected spectrum

The automated solution allows us and future users to evaluate its analytical reproducibility while minimizing reducible user bias and intervention. We anticipate the automated solution will help FT-IR researchers and data analysts to quickly and reliably analyze a large amount of data and connect them to a variety of available statistical learning methods to be applied to analyte absorbances isolated in atmospheric aerosol samples.

The authors acknowledge EPFL discretionary funding and funding from IMPROVE program and EPA (National Park Service cooperative agreement P11AC91045).

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