Atmos. Meas. Tech. Discuss.,
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Atmospheric Measurement Techniques Discussions

Interactive comment on "Analysis of functional groups in atmospheric aerosols by infrared spectroscopy: functional group quantification in US measurement networks" *by* Matteo Reggente et al.

Anonymous Referee #2

Received and published: 19 December 2018

General comments

This manuscript details the similarities and differences between peak fitting and partial least squares as means of interpreting the organic functional group composition of ambient aerosol. The work is appropriate for AMT and relevant to the scientific community as filter samples are a routine way to collect atmospheric particles. Further FTIR is a non-destructive technique, so this method can be paired with other methods of analyzing filter samples. This work builds upon recently published advances in the area of FTIR spectroscopy. The paper presents the quantitative comparison of two

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methods and provides sufficient detail for readers to understand the merits of partial least squares as an approach to FTIR analyses. All assumptions are clearly explained. In many cases, sensitivity type analyses are offered as well. The abstract provides a good summary of the article itself. The figures are of high quality and the table and figures are easy to read and understand. With the incorporation of minor suggested changes below, I support this manuscript for publication.

Specific comments

The title is satisfactory as written but does not indicate that the paper is primarily about the method of functional group quantification and not about the results themselves.

The manuscript is somewhat difficult to read, likely owing to the use of many acronyms and exhaustive detail of methods and results. In many cases, the authors could improve the readability of the manuscript by occasionally using the unabbreviated term (PLS, LVs, PF, etc) before returning to abbreviations.

Technical corrections

Pg 1 line 14: TOR used without definition

Pg 2 line 5: use “compose” instead of “comprise”

Pg 2 line 7: “methods . . .. include”

Pg 2, line 26: insert “and” before “ion chromatography”

Pg 11 line 15: I’m not sure if it should be “correspond” or “corresponds” please check the sentence meaning

Pg 11 line 31: I’m not sure what “evaluations of estimated quantities of using these absorption coefficients” means

Pg 13 line 23: define or redefine PFo and PFr

Pg 13 line 26: define or redefine PLSr and PLSbc

Pg 14 line 12: missing word “are thought to be an upper bound”

Pg 14 lines 13-14: awkward sentence “no evaporation loss of ammonium nitrate from PTFE or nitrate association with dust instead of ammonium are not considered”

Pg 14 line 25: do the authors mean “is likely”? Otherwise it is a double-negative

Pg 15 line 20: use “compose” instead of “comprise”

Pg 15 line 22: “vary” not “varies”

Pg 15 line 23: “correlation . . . is”

Pg 15 line 25: coefficient should be plural as it refers to two (14.84 and 8.89)

Pg 15 line 26: “correlation . . . is”

Pg 16 line 4: what is areal density?

Pg 16 line 27: I think the authors mean “such low abundances”

Pg 19 line 5: omit “a” before “another”

Pg 19 line 30: insert a space between “Phoenix, is”

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