

Interactive comment on “Analysis of functional groups in atmospheric aerosols by infrared spectroscopy: method development for probabilistic modeling of organic carbon and organic matter concentrations” by Charlotte Bürki et al.

Anonymous Referee #2

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The manuscript describes a novel approach using FT-IR and functional groups to obtain organic matter to organic carbon ratios. The manuscript fits the scope of Atmospheric Measurement Techniques. The data and approach are novel and appear of good quality. The manuscript could benefit from some attention to detail and some mostly minor clarifications.

A fundamental question that I do not see mentioned or addressed is that ATR spec-

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troscopy is highly sensitive to the deposit structure and depth homogeneity. I am missing a clear discussion on how the FG approach compares with PM mass? i.e. if the data gets less consistent with TOR when there is more deposit on the filter? Or not? This seems a critical thing to discuss?

A second related issue is what happens when diurnally different sources are important? E.g. vehicles AM and wood burning PM as the corresponding molecules are now in different layers and as stated above ATR is sensitive to penetration depth with higher sensitivity to molecules closer to the surface. Please comment? Could Phoenix data show something there?

Phoenix is being highlighted in the manuscript, which surprised me as I thought of IMPROVE being a rural network. In any case, even more surprising to me is the Phoenix woodburning. Can you please provide peer reviewed literature that actually supports that biomass burning is so dominant over the whole wintertime (3 months, if they have even 3 months of winter in Phoenix) and all this is not just some mass/deposit heterogeneity artifact as questioned above related to very strong inversion periods?

The manuscript could benefit from more attention to detail. Examples: L14 and throughout the manuscript-Please use subscripts in your molecule numbers. L14 COOH would be carboxylic acid especially when contrasted with carboxylate Figure 3: One molecule (dione) has carbons with 5 bonds (get rid of that double bond in the keto containing cycle). Also for all these species provide the correct names.. not only the random MCM naming. The second molecule is poorly cropped and cut.

Other comments: L19 R₂ values are meaningless without n? or discussion of statistical relevance., What is the “Reconstructed Fine Mass Equation”, I assume this is some American network thing? (L34) Blanks: why was only ammonium sulfate used as blanks? Not ammonium nitrate or other materials? Figure 2, could you provide quality parameters on the fits? Figure 5: Could you show a trendline with equation here? To get a quantitative idea of the drift? Figure 9: Probability density function are often given

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in units that if the curve gets integrated it equals 1. In this manuscript, it seems never normalized and the density always arbitrary? In Fig 9 on some panels one wonders if all areas under the curve are identical though?

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