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Atmospheric Measurement Techniques
Discussions
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Interactive comment on "Predicting ambient aerosol Thermal Optical Reflectance (TOR) measurements from infrared spectra: organic carbon" *by* A. M. Dillner and S. Takahama

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This is an interesting submission that aims to complete the chemical composition possible from a single Teflon filter, which is useful to air quality monitoring networks. The idea is that a single filter can be used to provide PM mass, metals (with XRF), BC (optical methods have been developed, but are not widely used), inorganic composition (destructive methods), and now with this manuscript, OC using non-destructive FT-IR. So it is very relevant to AMT.

However, I have one major concern. The authors have fixed the calibration data set at

2/3 of the field data. This is not the parameter I would have chosen to keep constant; it is also not how the real world application would work. That is because if to get the OC data from one hundred samples, I have to calibrate the technique with two hundred samples, then what is the cost advantage of using FTIR?

If I understand correctly, the calibration set is 2/3 of the field data set. That seems excessive, and significantly advantages the model. The authors find that when aerosol composition is different - higher OM/OC for test set than for calibration set, or apparently at Phoenix, where OM is less oxidized - the errors are higher. Figure 8 shows that the normalized error can be 20-25% at a single site (Olympic), even when data from all other sites is available to train the method, and the OC distributions are not significantly different between the calibration and test sets. This is even when the authors have two-thirds of the data set to train their model! What happens if samples are ordered at random, and the first one-third or or even first one-tenth of the samples are used for calibrating the method? What would be the errors and bias in the remaining test samples then? This is how I would expect the real world application to play out.

So in essence, the authors need to answer the question: Is an empirical calibration is required for each new data set, whether from a new site or a different year?

Minor subquestion: which type of spectra do the authors recommend, since they have evaluated three types?

Other specific comments:

Introduction - can skip some of the details of the two other details, because it is not clear those are relevant to the study at hand beyond “similar work has been done in other fields.” Ruthenberg et al. (2014) seems more relevant. But if R2014 already determined OM and OM/OC ratios with FTIR, doesn’t that lead to OC? So what’s new in this paper? The authors could help the reader understand the difference between R2014 and this submission, instead of discussing the two works from unrelated fields.

“inexpensive” - compared to TOR OC? Can the authors provide a relative estimate? TOR OC is direct, and only requires someone who can take a punch from a filter and stick it in a TOR oven - not very specialized tasks. FT-IR analysis appears much more specialized.

Why is OC mass for the blank filters assumed to be zero? The values are available from the monthly mean blanks.

Sec 2.4: “Evaluation of the quality of calibration” - I expected to actually see an evaluation of the calibration here, not just how the calibration is evaluated. The title should be revised to “methodology for evaluating the quality of calibration.”

Sec 3.3: “ammonium is often correlated with OC” - while this may be true for fairly regional/aged pollution, I would not expect it to be the case for urban environments. Second, the authors should provide references for this statement (which could also prove me wrong.)

If I understand correctly, the authors do not measure ammonium, but assume nitrate and sulfate exist as NH4NO3 and (NH4)2SO4. How good is this assumption across all sites?

Could the authors use TOR EC or an optical measure of BC from Teflon filters to perform a similar sensitivity analysis? The EC would be an indicator of the primary vs secondary nature of the sample aerosol.

Please clarify non-uniform cases - for example, the lowest 2/3 of what parameter predict the highest 1/3? Similarly for the other non-uniform cases.

The figures and analysis/write-up could be made simpler and direct by showing just one recommended spectra type (raw, baseline-corrected, or truncated), as the results do not significantly change based on spectra type. The discussion of the remaining spectra types can be relegated to the supplemental information for the very interested reader. What spectra type do the authors recommend?

Interactive comment on Atmos. Meas. Tech. Discuss., 7, 10931, 2014.

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