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Interactive Comment

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

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Anonymous Referee #1 Received and published: 14 August 2015 this Ms describes an alternative, non-destructive, way to obtain EC concentrations from (archived) PTFE filters collected by air monitoring networks. The method is described adequately (with reference to a companion paper dealing with obtaining OC concentrations) and the MS presents an exhaustive analysis of the performance of the method. Issues such as applicable concentration range, site differences etc are satisfactorily addressed. Whether this method is going to supplement or even replace the standard thermal optical determinanion of EC will be seen, but it is an interesting alternative and may

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have applications using archived filters.

Response: Thank you for your comments.

there are several cut-and-past remnants, typos and incomplete sentences, so I suggest to go through the MS again carefully.

Response: We have reviewed the paper carefully and corrected these errors.

Anonymous Referee #2 Received and published: 19 July 2015 General Comments: This paper describes a new method to measure elemental carbon (EC) in aerosol samples using FTIR. Measurements of aerosol EC are important because of its potential effect on human health, visibility, and global warming. The paper determines the best method for calibrating the FTIR measurements by using âĹij800 filter samples that have been collected at a variety of ambient sites. The FTIR method is calibrated by using partial least squares regression to correlate FTIR absorbance at a few characteristic wavelengths with standard thermal optical reflectance (TOR) measurements of EC for a selection of the samples and then the calibration is evaluated using the remaining samples. A very thorough evaluation is made of the potential chemical interferences to the FTIR method and effects of sample distribution and high and low EC loadings. The results indicate that FTIR can be used to make accurate measurements of EC, and it has the advantage of being inexpensive, rapid, and non-destructive. The measurements and data analysis are well done and the paper is clearly written.

Response: Thank you for your comments.

I have only one very minor comment, and otherwise think the paper should be published in AMT. Specific Comments: 1. Although a very thorough discussion is given regarding the potential chemical interferences to the FTIR method and effects of sample distribution and high and low EC loadings, I am still a little confused about exactly how, in practice, one should calibrate. I think the information is there in the Conclusions, but it could help to describe the procedure in a prescriptive, step-by-step manner.

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Response: The conclusion offers several options for developing the calibration and for the spectra type used. To provide one method that produced good results with our sample set, we have added text in supplemental material section S9. The reader is directed to this section in the conclusions. The following is the new supplemental material text.

S9. Calibration protocol In this paper, we show that several methods can be used to calibrate FT-IR spectra for accurate prediction of TOR EC using PLSR, so long as chemical composition of the calibration set spans the range of the chemical composition of the samples to be predicted. We summarize a canonical protocol for calibration and evaluation in this section. It is not necessary to baseline correct or modify the sample spectra produced by the FT-IR, beyond removing absorbance values arising from interpolation during the zero-filling process (which is done to reduce computational cost). We do not include blanks in the calibration model because for this data set, the inclusion of blanks did not impact the MDL calculation. However, blanks can be included as discussed in the methods section of the paper.

1. Select the calibration and test sets by ordering the samples by TOR EC mass and selecting every third sample for the test set and the rest of the sample for the calibration set.

2. Put the calibration set TOR data and raw spectra into a PLS model and select the model with the lowest RMSECV. This is called the Uniform EC calibration.

3. Order the samples in the lowest 1/3 of predicted FTIR EC range and put every third into the "low EC" test set and the rest into the low EC calibration set. Include blanks in the test set.

4. Develop a PLS model with the low EC calibration set and use it to predict the low EC test sets. This is called the Low Uniform EC calibration. Use the predictions from the Low Uniform EC calibration for the low EC test samples. Use the prediction of the blanks to calculate the MDL.

5. Use the predictions from Uniform EC calibration as the predictions for the rest of the samples.

Technical Comments: 1. Page 6326, line 21: “produces” should be “produce”. 2. Page 6328, line 7: Delete “they are” 3. Page 6328, line 17: “filters” should be ‘filter”. Response: These changes have been made.

Interactive comment on Atmos. Meas. Tech. Discuss., 8, 6325, 2015.

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