

Estimation of organic and elemental carbon using FT-IR absorbance spectra from PTFE filters

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Problem statement

Organic carbon (OC) and elemental carbon (EC) are major components of atmospheric PM. Typically OC and EC are measured using thermal optical methods from samples collected on quartz filters. However, these measurements are destructive and relatively expensive.

We aim at reducing the operating costs of large air quality monitoring networks using Fourier transform infrared spectra (FT-IR) of ambient PTFE filters and partial least square regression, as an alternative for quantification of OC and EC.

Contributions

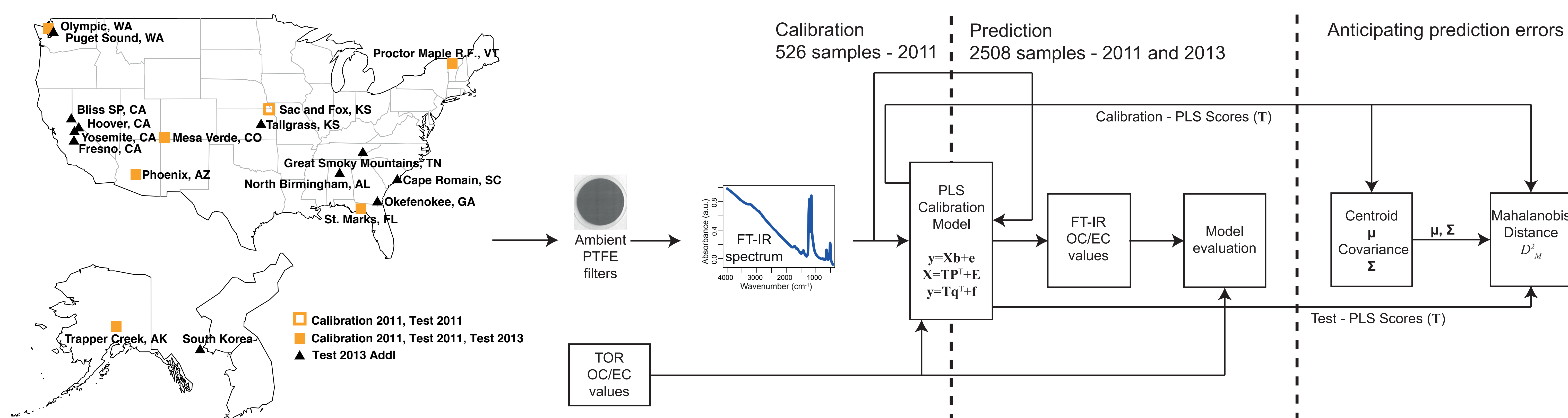
We achieve accurate predictions ($0.95 \leq R^2 \leq 0.97$) for models (calibrated in 2011) that use samples collected at the same sites of the calibration dataset but a different year (2013) (Results 1 and 4).

We demonstrate that spectral features contain information that can be used to anticipate prediction errors for OC and EC using a particular calibration model. We use the squared Mahalanobis distance to discriminate between sites that likely have predictions below or above pre-defined errors (Results 2 and 5).

We achieve accurate predictions ($0.91 \leq R^2 \leq 0.96$) for models (calibrated in 2011) that use samples collected at different sites of the calibration dataset and a different year (2013) (Results 3 and 6).

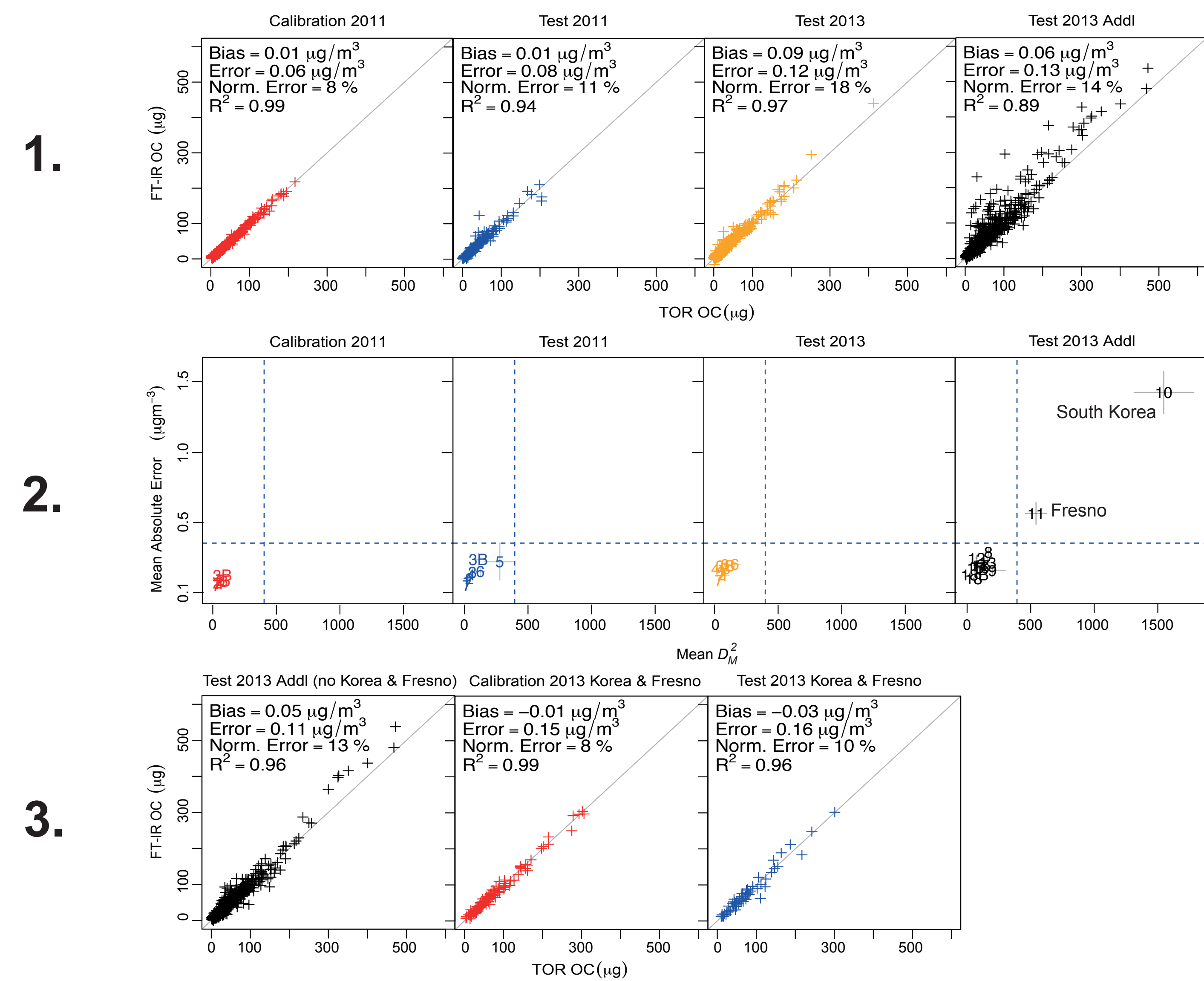
Sites with samples that are on average dissimilar to those in the calibration are shown to benefit from the construction of a separate calibration model (Results 3 and 6).

Methods



Results

FT-IR OC



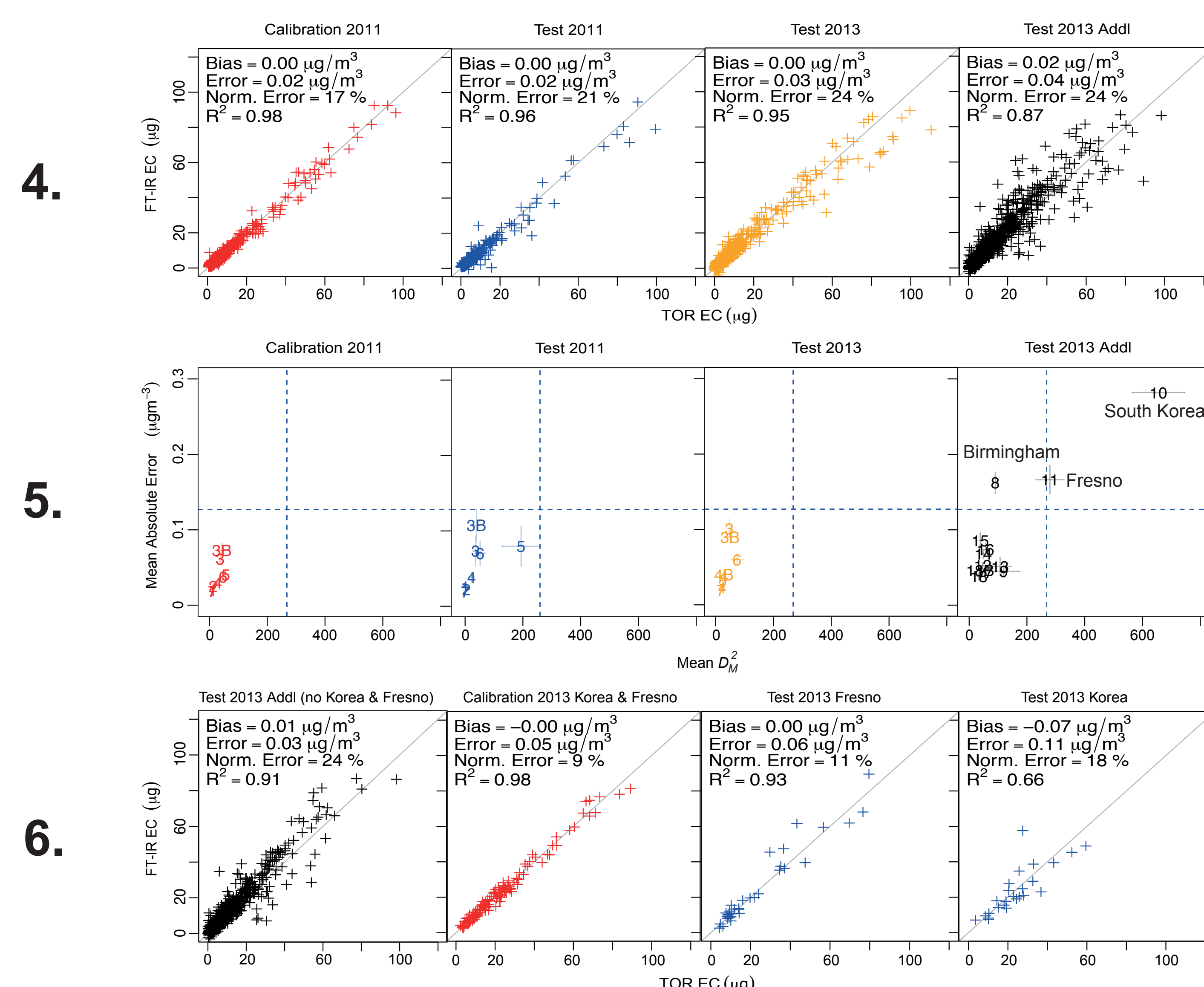
FT-IR and PLS accurately predict ($0.94 \leq R^2 \leq 0.97$) TOR OC values from PTFE ambient samples collected at the same sites and in the same or different years of the ones used for the calibration (blue and orange scatterplots).

Two sites in the Test 2013 Addl (black) have mean D_M^2 and mean absolute errors above the boundaries used for discrimination of unacceptable prediction errors (true positives). This two sites may contain different sources and chemical composition that are not well represented in the Calibration 2011.

Black: Test 2013 Addl without the samples collected at the two sites anticipated (and confirmed) to have high errors. The R^2 metric notably improves from 0.89 to 0.96.

Blue: accurate predictions ($R^2=0.96$), with a new calibration model (red), also at Fresno and Korea.

FT-IR EC



FT-IR and PLS accurately predict ($0.95 \leq R^2 \leq 0.96$) TOR EC values from PTFE ambient samples collected at the same sites and in the same or different years of the ones used for the calibration (blue and orange scatterplots).

Two sites in the Test 2013 Addl (black) have mean D_M^2 and mean absolute errors above the boundaries used for discrimination of unacceptable prediction errors (true positive).

The Birmingham site is misclassified (false negative).

Black: Test 2013 Addl without the samples collected at the two sites anticipated to have high errors. The R^2 metric improves from 0.87 to 0.91.

Blue (Fresno): accurate predictions ($R^2=0.93$), with a new calibration model (red).

Blue (Korea): the worse performance are mostly due to one sample, and the rest of predictions are more accurate (R^2 increases from 0.66 to 0.84).