Testing a new decrypted algorithm for Plantower sensors measuring PM2.5: comparison with an alternative algorithm.

Supplementary Materials

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S1.0 Historical progression to present-day PM2.5 and PM10 definitions.

Most clean air legislation today stems from the great London Smog of December 5-9, 1952, a result of a strong atmospheric inversion trapping industrial emissions of respirable particles, originally thought to have caused about 4000 deaths during those four days, but ultimately reassessed to an estimate of 12,000 excess deaths between December 1952 and March 1953 (Bell and Davis; Britannica 2022).

That same year, the British Medical Research Council (BMRC) defined respirable aerosol in terms of the probability (on average, for a population of typical human subjects and for ranges of typical breathing and physiological parameters), as a function of diameter, that an inhaled particle may penetrate to the alveolar region of the lung. The BMRC definition is described by a curve where the penetration probability falls from unity at a particle diameter near 10 um, passing through 50% at 5 um (Walton et al, 1998). Later, the 1968 curve of the American Conference of Governmental Industrial Hygienists (ACGIH), placed the 50% penetration probability at 3.5 um (Phalen 1988). The ACGIH defined PM10 and PM3.5 as follows:

> A PM10 sampling criterion was set for a particle size-selection device with efficiency described by a cumulative lognormal function with median (d_{50}) of 10 ± 1 µm aerodynamic diameter and with geometric standard deviation (σ_g of 1 .5 ± 0.1). Respirable samples were then recommended to be a device with size collection efficiency described by a cumulative lognormal function with median (d_{50}) of 3.5 ± 0.3 µm aerodynamic diameter and with geometric standard deviation *(*σ_g*)* of 1.5 ± 0.1).

In the 1990s, there was also international discussion at the Institute for Occupational Medicine (IOM) of the 50% cutoff for respirable particles and a value of 4 µm was selected. (Some current low-cost particle monitors manufactured in Europe include a 4- µm boundary for one of the size categories) (CEN (1993)) Size Fraction Definition for Measurement of Airborne Particles, European Standard EN 481: CEN European Committee for Standardization, rue de Stassart 36, B-1050 Brussels, Belgium. CEN 1995. Workplace atmospheres – Guidance for the assessment of exposure by inhalation to chemical agents for comparison with limit values and measurement strategy. CEN 689. European Committee for Standardization (CEN), Brussels.

Later, these health-based breakpoints of 3.5 or 4 um were revised by the US EPA to better divide particles into two classes based on separating smaller particles(often created as secondary organic aerosols) from the larger particles due to primary emissions and often having quite different chemical composition. The EPA determined that the best breakpoint separating the two classes would be 2.5 um. For optical particle sensors, there were thus three size categories for fine particles (PM2.5) (0.3-0.5 um, 0.5-1 um and 1-2.5 um) and two size categories (2.5-5 um, and 5-10 um) for "coarse" particles. PM10 is the sum of the fine and coarse particles. The 6th and final size category includes all sensed particles >10 um. These same 6 breakpoints are still used in many of the low-cost monitors available now.

Within six months of the establishment of the EPA, regulations were established for outdoor concentrations of Total Suspended Particulates (TSP) and PM10, later to be modified to focus mainly on PM2.5, with an annual standard today of 12 ug/m3 and a daily standard of 35 ug/m3. (These standards are presently in the process of being revised to lower levels, perhaps to 8 or 9 ug/m3 as an annual limit). All EPA standards are for outdoor air; EPA has no authority over indoor air, although it does support indoor air research. The WHO established an annual standard of 10 ug/m3 in 2005 but reduced that to 5 ug/m3 in 2021. This is an aspirational rather than a regulatory goal, since every one of the 100 most populous cities in the world exceeded an annual average of 5 ug/m3 in 2020 (https://www.greenpeace.org/static/planet4-international-stateless/2021/09/d93292fc-media-briefing_who-air-quality-guidelines).

S1.1 Development of optical particle monitors

Optical particle monitors were developed in the 1960s and 1970s []. These instruments use light scattering to detect, count, and size particles. Each particle produces a pulse in the detector, and the strength of the pulse can be used to size the particle, with larger particles producing stronger signals. Several portable instruments were developed for industrial hygiene use to estimate occupational exposure. The lower limit of sizes measurable by light scattering is about 0.3 μm, so the instruments of the 1970s and 1980s typically had 6 size categories with cutpoints at 0.5, 1, 3.5, 7, and 10 μm. (Note the cutoff of 3.5 μm, corresponding to the ACGIH curve) []. This value of 3.5 μm became a standard for OSHA workplace regulations of respirable particle concentrations. Early manufacturers of these instruments (e.g., Climet and Met One) used white light as the light source. Eventually, lasers replaced the white light as the light source, but the size categories remained the same for the instruments used in industrial hygiene applications. These particle counters were used in workplaces to estimate particle exposures and also in clean rooms to verify particle levels were below a given maximum.

Lasers made possible the development of more advanced optical particle counters, such as TSI's Model 3330 with 16 size categories between 0.3 and 10 um, and the Alphasense OPC Model N2 providing estimates of PM1, PM2.5 and PM10 from 16 bins ranging from 0.38 um to 17 um []. The Alphasense model N2 is considered a low-cost optical monitor at prices in the neighborhood of $500. This model was extensively analyzed in Crilley et al., (xxxx, xxxx). The Alphasense N2 provides considerable information on how it calculates mass from number counts. First it assumes a refractive index of 1.5 with no imaginary component. All particles are assumed to be spherical with a diameter D_p equal to the arithmetic mean of the upper and lower boundaries of each bin. Then the number N of the particles in one size bin is multiplied by the single-particle volume of $\pi D_p^3/6$ to calculate the total particle volume in each bin. This volume is then multiplied by a density of 1.65 g/ml to calculate the particle mass such as PM1, PM2.5 and PM10. The OPC-N2 is calibrated using Polystyrene Spherical Latex Particles (PSLs) of a known diameter and refractive index. Recognizing that the theoretical mass estimates may not apply to the real world, Alphasense also supports adding a correction factor to better approach measured values of reference instruments.

The TSI Model 3330 uses a similar approach in most respects to the Alphasense OPC N2. However, the midpoint of each size category is considered to be the geometric mean rather than the arithmetic mean of the boundaries. Also an arbitrary density of 1 g cm^{-3} is chosen with the recommendation that users select a density of the aerosol mixture as input into a final calibration factor. These two differences need to be factored in to any comparison of the devices. Note that the simple apparently minor change from using the geometric mean to using the arithmetic mean would itself account for a 27% increase in estimated PM2.5.

S1.2 Relationship of the two Plantower algorithms CF_1 and CF_ATM

We can determine the relationship between the two algorithms using about 7000 measurements made in a Santa Rosa home using a PurpleAir monitor PA-II with two Plantower PMS 5003 sensors. The relationship is shown in Figure S1.

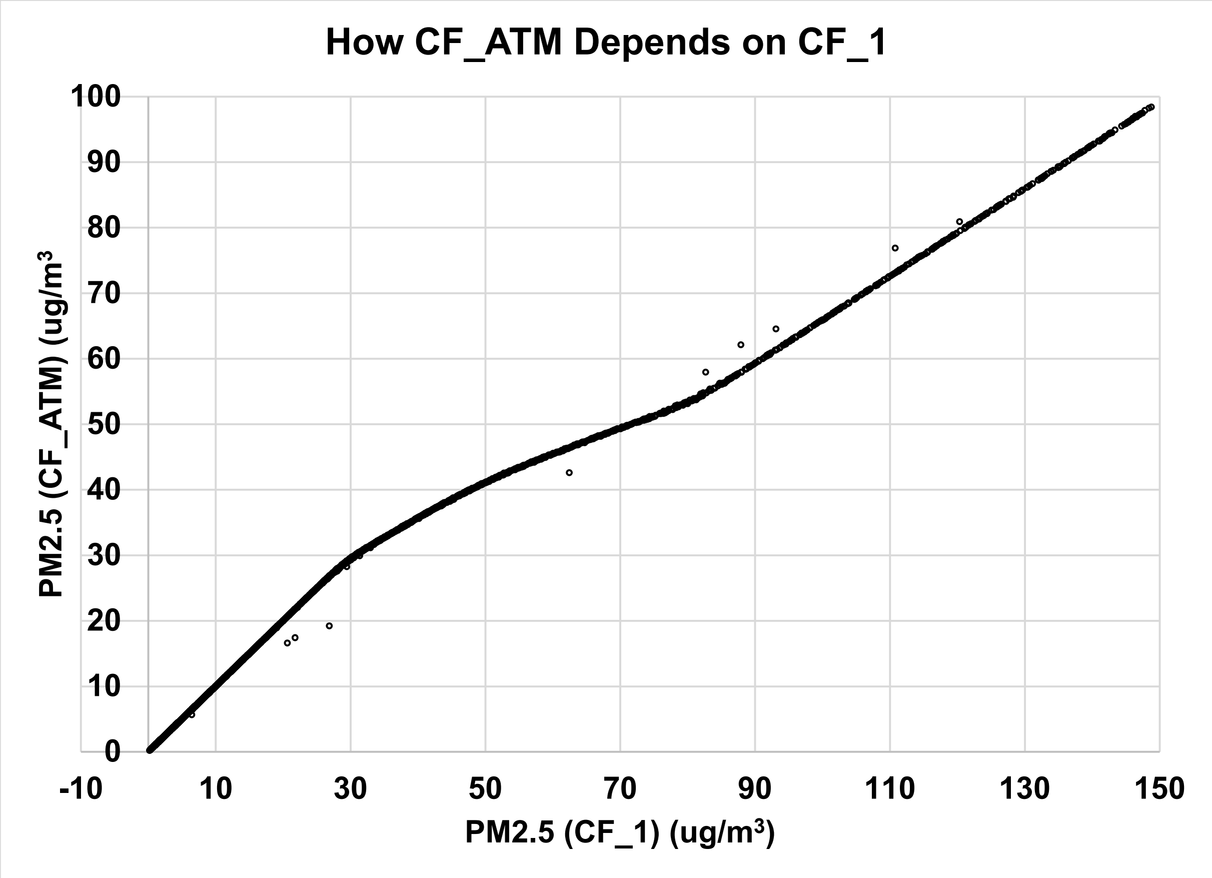

Figure S1. PM2.5 using the CF_ATM algorithm as a function of the same measurement using the CF_1 algorithm.

The direct relationship (ratio of CF_1/CF_ATM) is shown as a function of the concentration as measured in a 5-month study with >100,000 2-minute average measurements (Figure S2).

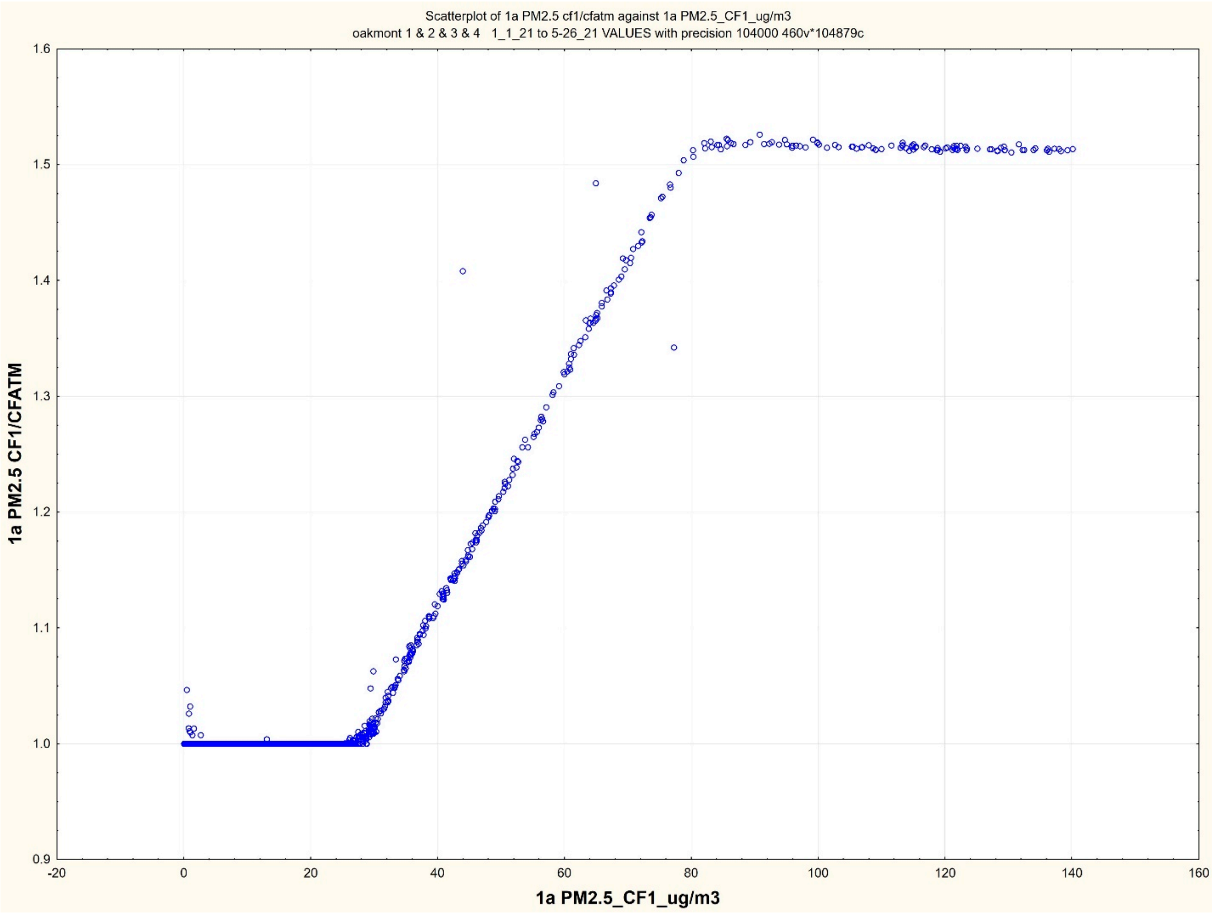

Figure S2. The ratio of CF1 to CF ATM as a function of CF1.

We see that the two algorithms give identical values (ratio of 1) below about 28 µg/m3. Then there is a linear increase in the ratio of CF_1 to CF_ATM out to about 78 µg/m3. Finally there is a constant ratio of about 1.5 at all higher concentrations. That is, if CF_1 is the correct algorithm, the CF_ATM algorithm matches it out to 28 ug/m3, starts falling below at that point until at 78 ug/m3 it has reached only 52 ug/m^3 (2/3 of the CF_1 value), and then magically corrects itself to stay at the 2/3 value out to hundreds of micrograms per cubic meter.

It is of course impossible for any physical relationship to behave in this manner. If one of the algorithms is correct, then the other is simply not based on physical reality. Selection of the more nearly correct algorithm has been done by comparing the two algorithms to measured data using research-grade or regulatory (gravimetric) instruments. These comparisons show linear relationships with CF_1 (Figure S3) and non-linear with CF_ATM (Figure S4), indicating that CF_1 may be the more nearly correct algorithm (Wallace et al., 2021). We conclude that CF_ATM is the problematic algorithm.

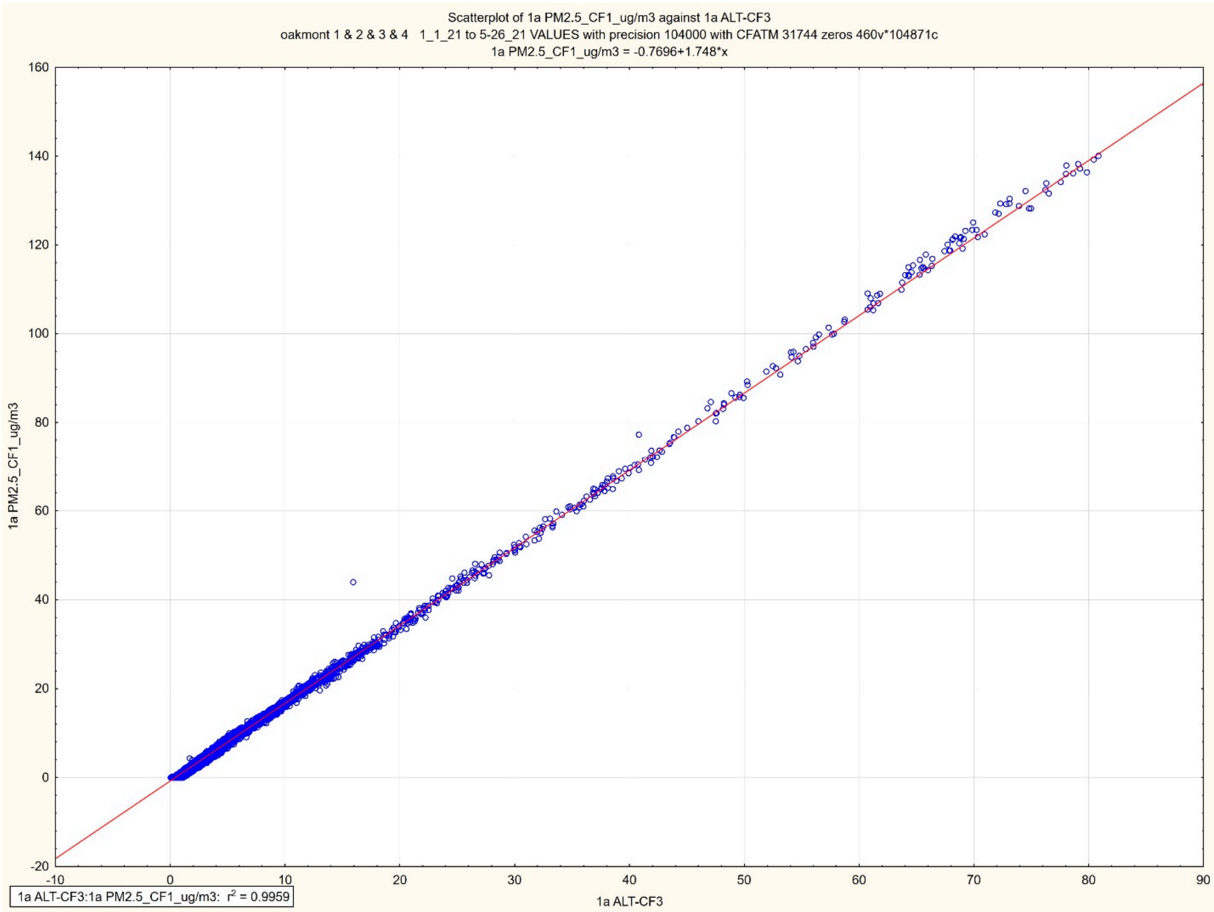

Figure S3. ALT-CF3 is highly correlated with CF1 (R2=0.9959), although CF1 overestimates PM2.5 by about 75% (slope of 1.748).

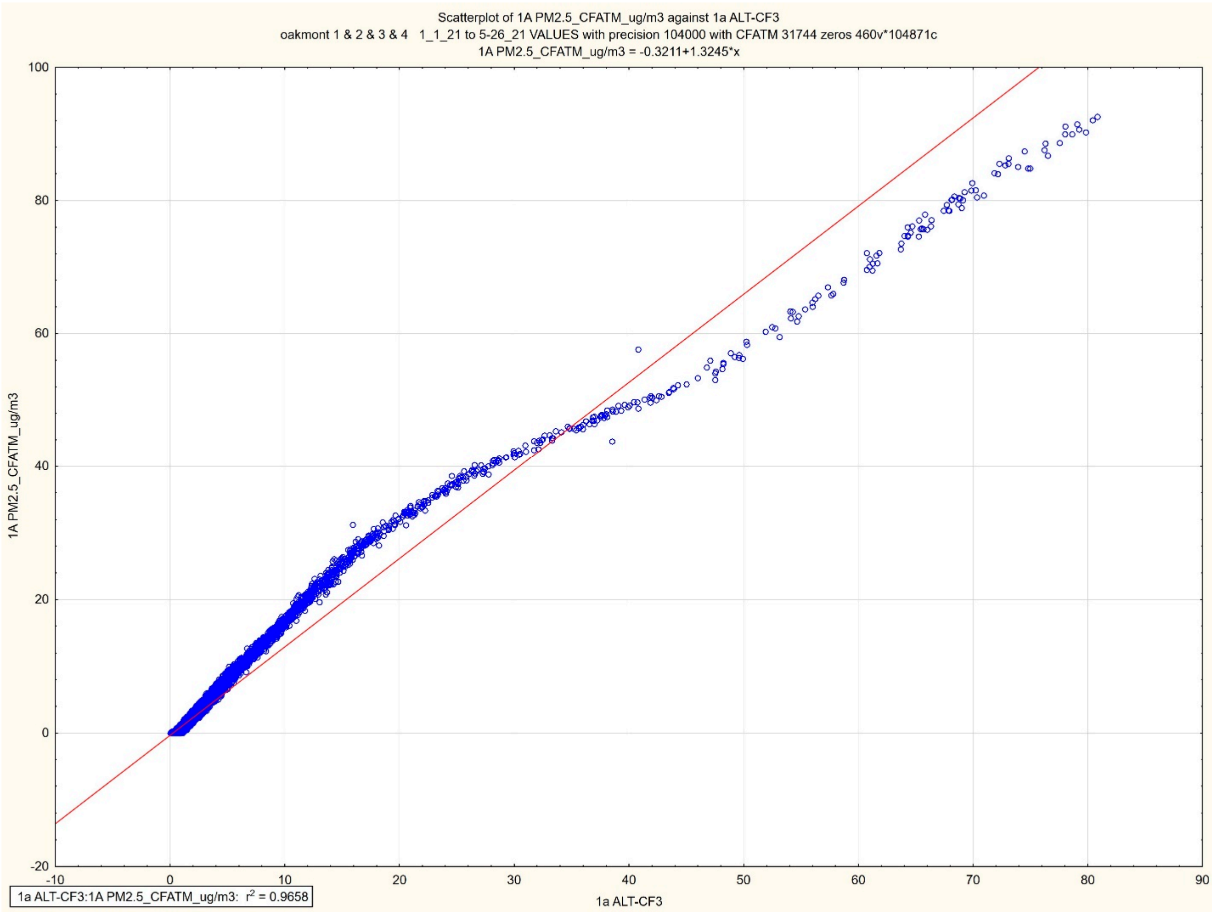

Figure S4. The CF ATM algorithm shows two inflection points at y-axis values of 28 and 52 ug/m3. (These correspond to CF_1 values of 28 and 78 ug/m3). The overall slope shows an overestimate of about 32%, which is less than the CF1 overestimate, but clearly distorted with respect to ALT-CF3.

S1.3 Redwood City results for 2021-2022 dataset

The 17-month dataset from Redwood City (4/29/21 to 9/27/22) is summarized in Table S1 for the three PA-II monitors 7, 8, and 9. Monitor 9 was outdoors.

Table S1. Basic statistics for Monitors 7, 8, and 9 in the Redwood City site.

Sensor	Valid N	Mean	Standard Error	Lower quartile	Median	Upper quartile	Maximum
7a	78938	4.08	0.037	0.76	2.2	5.0	670
7b	78938	3.77	0.037	0.62	2.0	4.6	680
8a	78935	3.77	0.027	0.59	2.0	4.6	459
8b	78935	4.23	0.028	0.76	2.4	5.5	473
9a OUT	78329	7.80	0.050	0.92	3.8	9.7	777
9b OUT	78328	9.51	0.050	3.02	5.8	11.3	819

The best individual models and resulting general model (highlighted) for the Redwood city data is provided in Table S2.

Table S2. Estimates of the coefficients a, c, and d for the individual models of CF_1 PM2.5 for the Redwood City site. Also estimates of the mean (or general) model (highlighted).

Sensor	a	c	d
7a	0.005057	0.079887	-0.93434
7b	0.004818	0.091025	-0.85203
8a	0.004058	0.096571	-0.85047
8b	0.003728	0.10318	-0.8238
9a OUT	0.00439	0.0804	-1.68901
9b OUT	0.004746	0.080991	-0.80517
mean	0.004466	0.088676	-0.99247
SD	0.000504	0.009829	0.344083
SE	0.000206	0.004013	0.140471
RSD	0.113	0.111	-0.347
RSE	0.046	0.045	-0.142
RSE(%)	4.6	4.5	14.2

Performance of the Redwood City individual best-fit models and the general model in estimating CF_1 PM2.5 observations is addressed in Table S3. The individual models approach the origin closely (maximum value of 0.048 ug/m3). Their slopes and R^2 values are above 0.99 in five of six cases. The general model also meets requirements for a good fit of a model to observed concentrations, with all intercepts less than 1 ug/m3 and all slopes between 0.95 and 1.065.

Table S3. Redwood City regression statistics for Individual and general models of the CF_1 algorithm: Number of observations, slopes, intercepts, and R^2 values for 6 independent PMS 5003 sensors.

		Individual models			General model		
Sensor	Valid N	Intercept (ug/m3)	slope	R^2	Intercept (ug/m3)	slope	R^2
7a	78938	0.0016	0.9997	0.9996	-0.1413	0.9932	0.9995
7b	78938	0.0026	0.9993	0.9993	-0.1942	0.9502	0.9993
8a	78935	0.0484	0.9871	0.9871	-0.04	0.994	0.9856
8b	78935	0.027	0.9935	0.9936	0.0513	0.9892	0.9907
9a OUT	78329	0.0244	0.9966	0.9963	0.7474	1.0646	0.9967
9b OUT	78328	0.0173	0.9982	0.9982	-0.3219	1.0242	0.9979

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