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From air quality sensors to sensor networks: Things we need to learn

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ABSTRACT

As a potential complement to traditional regulatory instruments, low-cost air quality sensors (LCAQS) can be deployed in dense monitoring networks to provide timely and comprehensive snapshots of pollutant concentrations and their spatial and temporal variability at various scales with relatively less cost and labor. However, a lack of practical guidance and a limited understanding of sensor data quality hinder the widespread application of this emerging technology. We leveraged air quality data collected from state and local monitoring agencies in metropolitan areas of the United States to evaluate how low-cost sensors could be deployed across the U.S. We found that ozone, as a secondary pollutant, is more homogeneous than other pollutants at various scales. PM_{2.5}, CO, and NO₂ displayed homogeneities that varied by city, making it challenging to design a uniform network that was suitable across geographies. Our low-cost sensor data in New York City indicated that PM_{2.5} sensors track well with light-scattering reference methods, particularly at low concentrations. The same phenomenon was also found after thoroughly evaluating sensor evaluation reports from the Air Quality Sensor Performance Evaluation Center (AQ-SPEC). Furthermore, LCAQS data collected during wildfire episodes in Portland, OR show that a real-time (i.e. *in situ*) machine learning calibration process is a promising approach to address the data quality challenges persisting in LCAQS applications. Our research highlights the urgency and importance of practical guidance for deploying LCAQS.

1. Introduction

Particulate Matter (PM), Ozone (O₃), Nitrogen Oxides (NO_x), and Carbon Monoxide (CO) have been linked to adverse effects on human health and are regulated as criteria air pollutants by the U.S. Environmental Protection Agency (U.S. EPA) [1–5]. Traditional, government-run air quality stations use instruments that meet the requirements of the U.S. EPA Federal Reference Methods (FRM) or Federal Equivalent Methods (FEM) for the monitoring of air pollutants [6,7]. These instruments tend to be bulky, expensive, and require rigorous standard operation procedures. While they are often feasible for use in limited settings around cities, they are insufficient to fully characterize the spatial distribution of air pollutants and their sources, especially within densely populated areas.

In the last decade, low-cost air quality sensors (LCAQS) have created a new era of air quality monitoring that leverages advances in the Internet of Things (IoT), digital electronics, and machine learning technologies. Due to their relatively low cost, ease of installation, and ability to provide continuous, real-time data, LCAQS can be deployed as part of dense monitor networks to provide a comprehensive picture of pollutant concentrations and spatial and temporal distributions of pollutants at various scales. One advantage of LCAQS is their capability to serve as the backbone of dense monitoring networks, allowing researchers, community groups, and regulatory agencies to understand better the air pollution sources, trends, and variations experienced by populations [8]. As an essential complement to traditional regulatory-grade instruments, LCAQS have been increasingly used for urban air quality mapping, fence-line/community monitoring, wildfires

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monitoring, and human exposure assessment [9–15].

Even though LCAQS have shown promising performance in several evaluations, they still face many challenges, especially regarding data quality. Numerous evaluation projects have assessed the performance of LCAQS in comparison with co-located regulatory-grade instruments. The U.S. EPA and the European Joint Research Centre (JRC) have also conducted field evaluations through several air monitoring projects [16–18].

In the ambient environment, the performance of PM and gaseous sensors are impacted by various factors, including signal drift, sensor lifetime, temperature and humidity effects, and interfering ambient compounds [19–23]. To overcome the synergy of those factors, machine learning algorithms have been leveraged to calibrate the sensors post-hoc [24–28]. The emergence of cloud computing has made real-time (i.e., *in situ*) calibration possible, even for a large network consisting of hundreds of air quality sensors [29–31]. However, the scientific community continues to debate appropriate methods for sensor evaluation, calibration, and how best to ensure long-term data quality after deploying air quality sensors.

Typically, evaluation of an LCAQS is conducted by comparing sensor data with the data from co-located regulatory monitors. The performance of LCAQS is assessed by several statistical indexes, such as coefficient of determination (R^2), slope (k) and intercept (b), root mean square error (RMSE), mean absolute error (MAE), and mean bias error (MBE) [32,33]. U.S. EPA recently published their recommended performance metrics and target values for $PM_{2.5}$ and O_3 LCAQS [34,35]. Several studies also attempted to evaluate the performance of the sensors by comparing the level of R^2 between sensors and reference methods [17]. For example, McKercher, Salmond [36] regarded the results of $R^2 > 0.75$ and slope close to 1.0 as a good level of performance. However, there can be a systematic error that varies from one type of reference method to another. Zheng, Bergin [37] reported that $PM_{2.5}$ (PM with aerodynamic diameters less than $2.5 \mu m$) from LCAQS compared better with the Teledyne API T640 PM mass monitor (T640), a US EPA Federal Equivalent Method (FEM), than with the β -attenuation-based monitor (E-BAM-9800, Met One Instruments), another research-grade measurement method (non-FEM designation).

In addition to the type of reference monitor used for calibration, the optimal density of an LCAQS network is still a subject of research and is related to the question of the homogeneity or heterogeneity of regional ambient air pollution. Numerous studies have investigated the spatial homogeneity of air pollutants [38–40]. Faridi, Niazi [38] reported the highest homogeneity for $PM_{2.5}$ and NO_2 in Tehran, Iran, which was attributed to traffic-related emissions in different districts. Chow, Chen [39] reported that the representativeness of $PM_{2.5}$ measurements changed from 5–10 km in the urban areas to 15–20 km in the boundary and rural regions after investigating over one-year of data from 38 sites across the central California region. However, most of these analyses focused on one or two pollutants with data from sites in a single city/region.

Furthermore, calibration methods for LCAQS typically follow a procedure. First, data are collected from LCAQS dispersed across an area. One or many of these LCAQS are co-located with reference grade instruments, either once or periodically to establish a calibration. Based on the calibration, corrections are then applied to all data post-collection to standardize the LCAQS measurements to reference methods. If not conducted frequently enough or based on a short period of time, this procedure may fail to capture events that lead to changes in calibration, such as wildfires, resulting in inaccurate reported concentration.

In this paper, we describe our experience from recent LCAQS field evaluations and discuss insights from managing a LCAQS network. Specifically, we present three case studies to explore the following questions: 1) Does the optimal density of LCAQS vary by location and pollutant of interest? 2) Is every reference method equivalent for calibrating LCAQS? 3) Does calibration using an *in situ* machine learning

algorithm perform better than conventional post-processing methods?

2. Data and methods

2.1. EPA air quality data

All outdoor regulatory monitoring data included in this research were obtained through the EPA Air Quality System (AQS) application programming interface (API) (https://aqsweb/documents/data_api.html). For every air pollutant ($PM_{2.5}$, O_3 , CO, and NO_2), EPA air quality monitoring sites (referred to as “EPA sites” throughout this paper) with available measurements by FEM/FRM methods from 2017 to 2019 were first identified by evaluating daily data during that period. The distances between each pair of these available sites were calculated based on the longitude and latitude coordinates provided by the EPA site list (Table S1). PM_{10} (PM with aerodynamic diameters no more than $10 \mu m$) and SO_2 were not included due to the lack of qualified sites and low concentrations throughout the country, respectively. Estimates of R-squared (R^2) between each pair of nearby EPA sites in twenty-one metropolitan areas across the U.S. (Fig. S1) were calculated versus their distance to explore the homogeneity of various pollutants. Those pairs of EPA sites with distance between each other < 10 km were selected for correlation analysis. Next, the ordinary least square (OLS) linear regression results were sorted by their associated core-based statistical area (CBSA). R^2 versus distance was then plotted separately for each of the CBSA areas containing three or more pairs of EPA sites within 10 km range. Unlike the previous spatial studies mentioned above [38–40], our analysis is at the national level covering four criteria air pollutants ($PM_{2.5}$, O_3 , CO, and NO_2) from a large number of sites across the U.S. (a total of 162 sites in 22 areas are described in Fig. 1 and Table 1).

2.2. SCI-608 sensor data at Queens College II site

We utilized the SCI-608 (SailBri Cooper Inc, Tigard, Oregon, USA) as a LCAQS; it is designed to measure six ambient air pollutants ($PM_{2.5}$, PM_{10} , O_3 , CO, NO_2 , and SO_2) and two related meteorological parameters (temperature and relative humidity) simultaneously with four electrochemical gas sensors (B4, Alphasense, UK), one laser particle sensor (PM2005, Cubic Sensor and Instrument Co., China), and one meteorological sensor (SHT21, Sensirion). A similar product has been used and described in detail in previous studies [15,41,42]. To adjust for the impact of environmental parameters on sensor output (e.g., gaseous cross-interference, temperature and relative humidity effects on gaseous sensors, and relative humidity’s impact on the PM sensor), the raw sensor data is processed by a machine-learning based calibration model (based on Least Absolute Shrinkage and Selection Operator (LASSO) regression algorithm, see Part 3 of the SI for more information); the resulting dataset is referred to as the “LCAQS output.” There are multiple common machine learning algorithms (including multivariate regressions, gradient boosting, XGBoost, artificial neural network, etc.) loaded on the SailBri Cooper cloud server, which dynamically chooses an optimal algorithm to calibrate each of the LCAQS. Both LCAQS raw data and processed outputs are saved on the server.

Two SCI-608 sensors were installed at the EPA Queens College II site (AQS ID: 36-081-0124, Fig. S1) in the city of New York, NY, and were co-located with two $PM_{2.5}$ FEM monitors – a Thermo Scientific 1405-DF tapered element oscillating microbalance monitor (TEOM) and a Teledyne API T640 PM mass monitor during summer of 2020. Both $PM_{2.5}$ FEM monitors were housed in a weather-controlled shelter and operated by the New York State Department of Environmental Conservation (NYSDEC). Two SCI-608 were sited on the rooftop of the shelter and close to the FEM PM inlets.

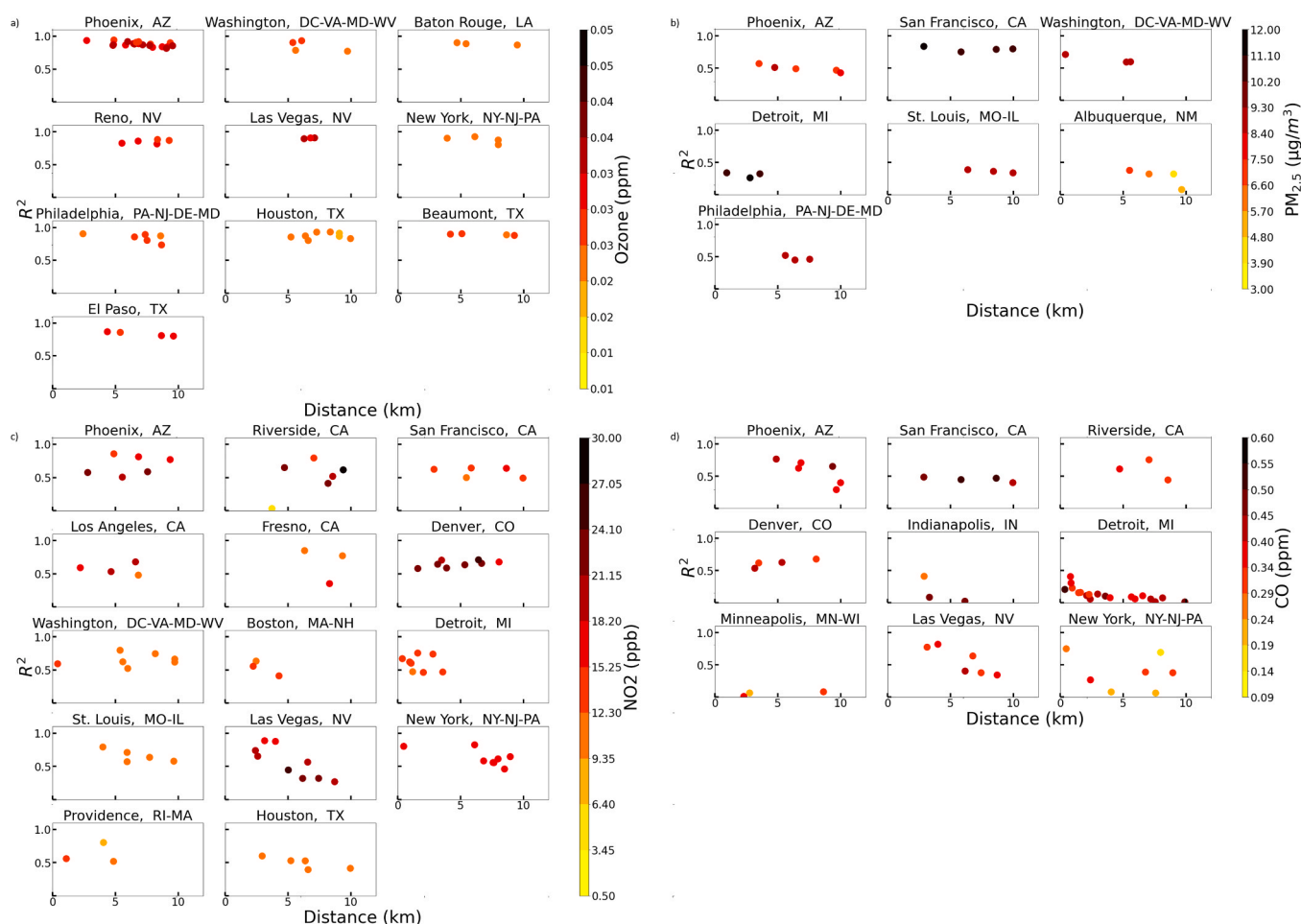


Fig. 1. R-squared (R^2) between each pair of nearby EPA sites versus their distance for (a) O₃, (b) PM_{2.5}, (c) NO₂, and (d) CO. The R^2 results were based on all available 1-hour data from 2017 to 2019, and the color bar indicates means of all available 1-hour concentrations from the paired sites for the period. Please refer to Table S1 for more details of CBSA.

2.3. SCI-608 sensor data during the wildfire episodes

During 2018, two SCI-608 were co-located alongside a reference-grade nephelometer (Radiance Research M903, light scattering principle) at the SE Lafayette site in Portland, Oregon (AQS ID: 41-051-0080, Fig. S1). After the first week of installation and calibration, the two sensors captured intermittent episodes of poor air quality due to wildfire smoke indicated by significant increases in PM_{2.5} and CO concentrations. The data presented here demonstrate the performance of the sensor against co-located reference methods during the wildfire episodes from August 2 to September 14, 2018.

3. Results & discussion

3.1. Does the optimal density of LCAQS vary by location and pollutant of interest?

Fig. 1 and Table 1 indicate that the correlation (R^2) varied with distance for pollutants measured at EPA sites in each metropolitan area (see Table S1). The R^2 between two sites was expected to decrease with increasing distance. When the distance equals zero, two instruments are co-located side by side and the R^2 (the determination of correlation between two co-located FEM/FRM instruments) is expected to be 1. Therefore, we performed OLS linear regression of R^2 versus distance by forcing the y-intercept (R^2 at a distance equals to zero) to be 1. For each pollutant in each metropolitan area, the slopes (k) with 95% confidence interval (CI), the R^2 of the regression result of the R^2 versus distance

(henceforth refer to as the R^2 of Reg), and the standard error of the regression (std. error) are listed in Table 1; the mean concentration in the CBSA (Mean Conc.) and regression p-value (p-value) are listed in Table S2. A regression p-value less than 0.05 ($p < 0.05$) would indicate that k is significantly different from 0. k has the unit of km^{-1} , representing the change in R^2 value per kilometer increase in the distance between the measurements at paired sites. The R^2 of Reg evaluates the linearity between the R^2 of paired sites versus their distance apart. The larger R^2 of Reg suggests a greater linearity, and so the slope (k , listed in Table 1) can more reliably predict the decay in R^2 between the measurements of two sites with the distance between the two sites. Standard errors indicate the averaged distance between data points and the regression line. Typically, a small standard error means the data points are close to the regression line and thus a good fit. In general, as a secondary pollutant formed in the atmosphere through chemical reactions, O₃ exhibited more spatial homogeneity than other pollutants. In Fig. 1(a), even at distances of ~ 10 km, O₃ data from two monitor sites still displayed a strong positive correlation with little variation as the distance increased (the k from -0.02 to -0.01 and values of the R^2 of Reg from 0.84 to 0.98). Since PM_{2.5} was often derived from different sources (primary and secondary), it displayed similar trends of homogeneity as O₃ with small variations in most of the urban areas (the k from -0.09 to -0.03 and values of the R^2 of Reg from 0.88 to 0.98). However, a weaker correlation among PM_{2.5} sites was found in the city of Detroit, MI, St. Louis, MO, and Albuquerque, NM. For instance, in Detroit, MI, even though the two sites were about 1 km away, PM_{2.5} data only showed a moderate correlation ($R^2 \sim 0.4$). Pinto, Lefohn [43] also found

Table 1

The summary of the slope (k) with 95% confidence interval (CI), R^2 of the regression (R^2 of Reg), and standard errors of the regression (std. error) of two EPA sites' R^2 versus their distances plotted for each CBSA in Fig. 1.

CBSA	PM _{2.5}			Ozone			NO ₂			CO		
	Slope (km ⁻¹)	R ² of Reg	Std. Error	Slope (km ⁻¹)	R ² of Reg	Std. Error	Slope (km ⁻¹)	R ² of Reg	Std. Error	Slope (km ⁻¹)	R ² of Reg	Std. Error
Phoenix, AZ	-0.067 ± 0.026	0.926	0.00943	-0.017 ± 0.0019	0.951	0.0009	-0.044 ± 0.033	0.700	0.01289	-0.055 ± 0.015	0.944	0.00597
Riverside, CA							-0.061 ± 0.052	0.646	0.02031	-0.057 ± 0.053	0.916	0.01227
San Francisco, CA	-0.027 ± 0.018	0.882	0.00563				-0.057 ± 0.028	0.887	0.0102	-0.071 ± 0.046	0.890	0.01433
Los Angeles, CA							-0.075 ± 0.055	0.864	0.01718			
Fresno, CA							-0.043 ± 0.078 *	**	**			
Denver, CO							-0.060 ± 0.028	0.787	0.01178	-0.064 ± 0.062	0.782	0.01959
Washington, DC-VA-MD-WV	-0.076 ± 0.10 *	**	**	-0.023 ± 0.015	0.882	0.00479	-0.043 ± 0.026	0.737	0.01055			
Indianapolis, IN										-0.19 ± 0.14	0.945	0.03209
Baton Rouge, LA				-0.017 ± 0.010	0.961	0.00236						
Boston, MA-NH							-0.15 ± 0.068	0.978	0.01576			
Detroit, MI	-0.24 ± 0.31 *	**	**				-0.18 ± 0.096	0.743	0.04049	-0.15 ± 0.047	0.726	0.02237
Minneapolis, MN-WI										-0.15 ± 0.30 *	**	**
St. Louis, MO-IL	-0.075 ± 0.034	0.979	0.0078				-0.050 ± 0.013	0.965	0.0048			
Albuquerque, NM	-0.091 ± 0.022	0.982	0.00706									
Las Vegas, NV				-0.014 ± 0.0048	0.988	0.00112	-0.086 ± 0.019	0.932	0.0082	-0.075 ± 0.018	0.959	0.00691
Reno, NV				-0.019 ± 0.0077	0.920	0.00276						
New York, NY-NJ-PA				-0.019 ± 0.0096	0.928	0.00303	-0.052 ± 0.013	0.932	0.0053	-0.093 ± 0.057	0.722	0.02346
Philadelphia, PA-NJ-DE-MD	-0.080 ± 0.022	0.992	0.00517	-0.022 ± 0.0080	0.911	0.00313						
Providence, RI-MA							-0.088 ± 0.18 *	**	**			
Houston, TX				-0.016 ± 0.0060	0.841	0.00255	-0.075 ± 0.026	0.942	0.00936			
Beaumont, TX				-0.015 ± 0.0065	0.946	0.00205						
El Paso, TX				-0.023 ± 0.0056	0.983	0.00174						

Note: Results with p-values greater than 0.05 are marked with “*” to indicate less than 95% probability and are excluded from discussions in Section 4.1. The R^2 of Reg and standard errors are not calculated for these CBSA with high p-values (p-value > 0.5), which are marked with “**” and excluded from the averaged R^2 of Reg and averaged standard error calculations in the context. All blanks in Table 1 are due to lack of data.

similarly varied spatial heterogeneity of PM_{2.5} in metropolitan areas across the U.S. and attributed it to several reasons such as varied local sources, different transient emissions events, etc.

In contrast, the primary pollutants CO and NO₂ exhibited more varied spatial heterogeneity with R^2 values decreasing substantially with distance in most urban areas. The k for CO and NO₂ were generally more negative than those of O₃ in almost every urban area, indicating the quick decrease in correlation as the distance increases. In addition, the spatial heterogeneity of CO and NO₂ varied widely in different geographies. For instance, the k was -0.057 and -0.071 for NO₂ and CO, respectively, within 10 km in San Francisco, CA. Meanwhile, the same value was -0.18 and -0.15 in Detroit, MI. In addition, the average R^2 of the Reg were 0.843 and 0.861 for NO₂ and CO, respectively, lower than the value for O₃ (0.931) and PM_{2.5} (0.952). These lower values indicate that the decreases in R^2 between sites for both NO₂ and CO over increasing distances result in less accurate predictions. Similarly, the average standard errors were 0.0139 and 0.0171 for NO₂ and CO, respectively (compared to PM_{2.5} (0.00702) and O₃ (0.00244)), suggesting more diverse from the regression line. As described in more

detail in the SI, the more diverse spatial heterogeneity of CO and NO₂ in some metropolitan areas may be attributable to the impacts of local climate, topography, or emission sources.

Thus, the extent of the homogeneity of air pollutants should be taken into consideration while designing the LCAQS network, both in terms of specific pollutants measured and density of the monitoring network to adequately capture heterogeneity in concentrations and enable either periodic or continuous calibration of LCAQS. Our results indicate that O₃ observations at a monitoring site could represent the surrounding concentration within a 10 km range. If we only consider designing an O₃ sensor network, LCAQS and EPA regulatory monitors would best be placed ~10 km apart in most metropolitan areas.

Our results suggest the design of the LCAQS network should thus be based on the requirements of what pollutants need to be monitored and what is known about the homogeneity of local environments. For instance, to build an LCAQS network to monitor PM_{2.5}, O₃, CO, and NO₂, in Phoenix, AZ, monitors should be installed within 5 km from one another. Meanwhile, in Detroit, MI, we recommend this distance to be ~1 km. Due to insufficient data, we could only conduct our analysis in

limited metropolitan areas. Local and federal government agencies – along with the research community and modelers – should conduct more investigations to appropriately determine the optimal sensor distance and density. In addition, since this conclusion is based on linear regression analysis, it is generally more reliable for PM_{2.5} and O₃, which have higher R² of Reg and lower standard errors compared to NO₂ and CO.

While operating an LCAQS network, it is crucial to ensure the quality of sensor data. Conducting periodic sensor calibrations by co-locating

the sensor with a reference site has been proven an effective approach [27,44,45] and has also been recommended by governmental monitoring guidances [46,47]. However, in some cases, due to challenges in accessing regulatory sites, we were only able to deploy LCAQS near reference station to finalize calibration. The use of mobile or portable reference or reference-grade instrumentation may be another cost-effective method for calibrating LCAQS [48,49]. For government agencies – whether national, state, or local – temporally deploying additional mobile or portable reference monitors along with LCAQS can

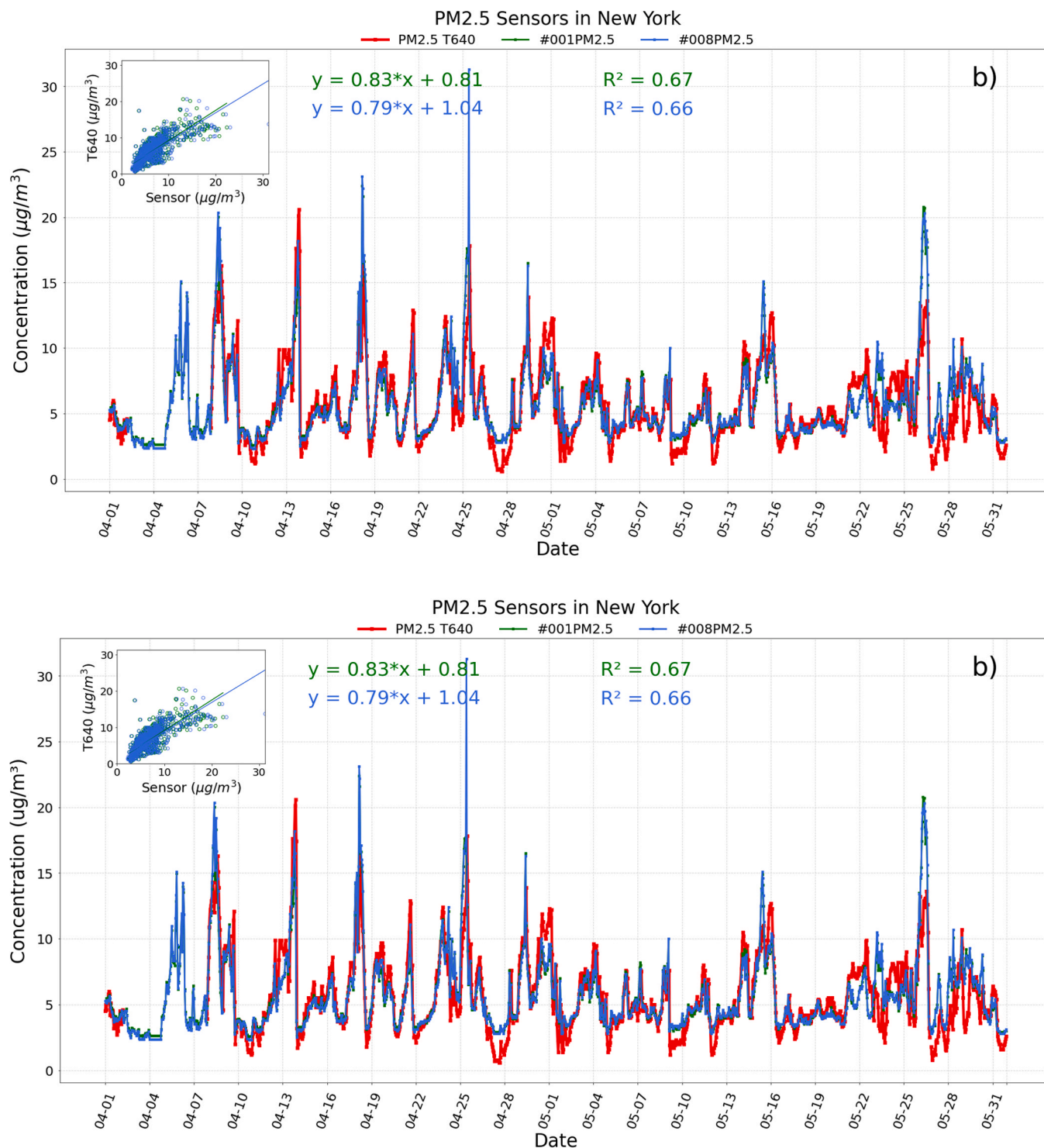


Fig. 2. Comparison between (a) hourly PM_{2.5} sensors and TEOM data with the inset panel showing the correlation between TEOM and each of the two sensors, and (b) hourly PM_{2.5} sensors and API T640 data from April 1 to May 31, 2020 with the inset panel showing the correlation between T640 and each of the two sensors.

facilitate calibration while also providing the benefit of increased spatial density of their networks. Finally, we note that monitors placed in non-spatially optimal patterns may still provide useful information on variability in a given geography, identifying pollution hotspot, as shown in earlier studies [50,51].

3.2. Is every reference method the same for calibrating LCAQS?

Fig. 2(a) and (b) show the comparison of $PM_{2.5}$ data between the SCI-608 sensors and two types of FEM methods (TEOM and T640), respectively, from April 1 to May 31, 2020. During our co-located observations, PM data from two SCI-608 showed a good correlation ($R^2 = 0.98$) with low RMSE, MAE, and MBE (Table S3). The two SCI-608 units' $PM_{2.5}$ sensor data displayed a better correlation with T640 (average $R^2 = 0.67$) than with TEOM (average $R^2 = 0.44$). The TEOM data showed small but significant fluctuations at $PM_{2.5}$ concentrations below $5 \mu\text{g}/\text{m}^3$, which we believe is the primary reason for the lower correlation. Additional comparisons, including time-series data and intercorrelations between two co-located SCI-608 units and intercorrelations between a TEOM and T640 are shown in Fig. S2. The large MBE/MAE ratio (0.84) between the T640 and the TEOM $PM_{2.5}$ measurements indicates that the biases are primarily one-sided, which we interpret as systematic bias rather than noise/random error, as random biases tend to appear on both sides by nature [32]. Such systematic bias also appears between the sensor and TEOM measurements (as indicated by the large MBE/MAE ratios (0.79 and 0.80) in Table S3), which contributed to the inconsistent results between the sensor and TEOM.

We observed similar phenomena in PM sensor evaluation results reported by the Air Quality Sensor Performance Evaluation Center (AQ-SPEC) at South Coast Air Quality Management District (South Coast AQMD). AQ-SPEC has continuously evaluated gaseous air quality and PM sensors under the same evaluation protocol in Riverside, California [32,33,52,53]. Their works filled the knowledge gap and provided invaluable references for the LCAQS community. AQ-SPEC conducts a systematic field PM LCAQS evaluation (Fig. S1) by co-locating triplicate PM LCAQS with two or three FEM methods (Teledyne API T640, Grimm EDM 180, Grimm Aerosol and BAM-1020, Met One Instruments) for nearly 8 weeks [52]. AQ-SPEC reports the correlation (R^2) between the sensor and co-located FRMs/FEMs concentrations. The R^2 values reported in AQ-SPEC's field evaluation reports are compared between FEM methods to gain insights into the differences in sensor performance resulting from the FEM method utilized for comparison. As of May 2020, there had been a total of 43 field reports, 31 of which compared the results of PM sensors between the BAM and Grimm (shown in Fig. 3a), and 11 of which compared the results of BAM and T640 (shown in

Fig. 3b). Even though the $PM_{2.5}$ sensors came from different manufacturers and models, these evaluation results suggest a better correlation of the sensors with the Grimm/T640 methods (light scattering principle) than with the BAM.

This evaluation indicates that $PM_{2.5}$ sensors tend to have better correlations with FEM methods with optical light scattering principles (such as Grimm 180 and API T640) than other FEMs (BAM and TEOM). Our results imply that there are inconsistencies between different types of FEMs, which can influence public assessment of sensor performance when simply comparing statistical results between data from LCAQS and unspecified reference or equivalent methods.

3.3. Does in situ calibration improve the LCAQS efficacy?

The machine learning method employed by the data management system for the SCI-608 sensors leverages historical data to optimize a prediction model, which then calibrates data reported by LCAQS. Several studies have shown that machine learning methods can enhance the data quality of LCAQS [26,54,55] when compared to traditional calibration methods. With the IoT technology, SCI-608 monitors utilize the calibration model (based on LASSO, see more details in SI) that are fully adapted on a cloud platform to conduct *in situ* calibration for LCAQS data. After the calibration, SCI-608 monitors can be deployed to any location of interest. The purpose of the constant co-location of SCI-608 with the reference method in this study was to assess the performance of LCAQS.

During the wildfire period, the sensor reported concentrations that were substantially higher than the concentration data used in the 1st calibration (over the maximum of the 1st calibration dataset by more than 100% of this dataset's range), which introduced the risk of over-extrapolation if the model continues using the previous calibration to predict the concentrations during the wildfire period. An over-extrapolation alarm was flagged in the cloud, and the two sensors then underwent an additional 24-hour calibration during the wildfire episodes on August 14. This "on-demand" calibration added co-located data to the previous calibration dataset and extended the range of the prediction model. The data presented here shows the performance of the sensor during the wildfire episodes from August 2 to September 14, 2018. Although in this demonstration the sensors were kept co-located with the reference method over the entire period, in real-world practices, sensor monitors can be located at any location of interest after their initial calibration. The additional, on-demand calibration can be accomplished by using a portable mobile reference monitor to co-locate with the sensors. Such a calibration can accommodate periods with atypical concentrations, like wildfires (as shown here), industrial releases, dust storms, etc.

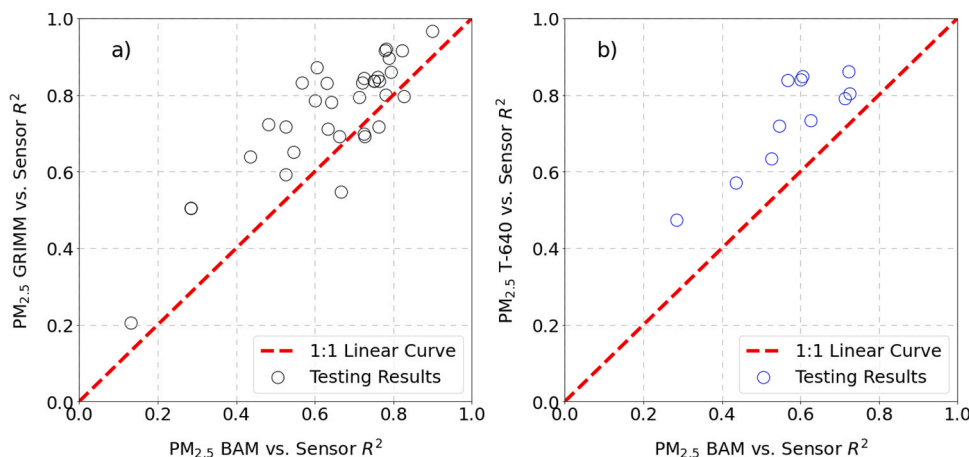


Fig. 3. Coefficient of determination (R^2) between sensors and different type of reference methods as (a) a comparison between GRIMM and BAM, and (b) a comparison between T640 and BAM.

Fig. 4 shows hourly averaged data from a reference method (Radiance Research M903) and from an LCAQS for PM_{2.5} concentrations during the wildfire season of 2018, in which two wildfire episodes were observed between 08/14/2018 and 08/22/2018. The maximum 24-hour values of PM_{2.5} are 81 $\mu\text{g}/\text{m}^3$ and 87 $\mu\text{g}/\text{m}^3$ in each episode – more than double the EPA 24-hour PM_{2.5} standard (35 $\mu\text{g}/\text{m}^3$). Although the sensors reported good results after the initial calibration (from 9 PM on August 2–9 PM on August 8, GMT) and before the wildfire episode (marked as “After 1st Calibration” in Fig. 4), neither sensor accurately captured the temporal variations in PM_{2.5} concentrations during the first wildfire episode on August 13–16. The reported concentrations were significantly higher than the concentrations during the initial calibration, which introduced the risk of over-extrapolation of the model. The maximum of the 1st calibration dataset (uncalibrated sensor reported data) was 30.2 $\mu\text{g}/\text{m}^3$ and the range was 30.0 $\mu\text{g}/\text{m}^3$ (maximum-minimum). After 11 PM on August 13 (GMT), there were more than 12 consecutive hours with raw measurements greater than the calibration dataset maximum plus 100% of the calibration dataset range (30.2 + 30.0 = 60.2 $\mu\text{g}/\text{m}^3$). As such, an *in situ* calibration alarm was flagged in the management system to notify the network operator to perform an additional calibration. This additional round of calibration added 24 h of co-located data, through 1-day temporary co-location during the first wildfire episode (from 12 AM August 14–12 AM August 15, GMT), on top of the previous calibration dataset for machine learning, resulting in the sensors’ performance being improved for the second wildfire episode (from August 15 to September 14) with the averaged RMSE decreased from 4.46 $\mu\text{g}/\text{m}^3$ to 3.83 $\mu\text{g}/\text{m}^3$ and MAE decreased from 2.50 $\mu\text{g}/\text{m}^3$ to 2.21 $\mu\text{g}/\text{m}^3$ (Fig. 4 and Table 2). As the additional calibration extended the range and maximum of the calibration dataset, the *in situ* calibration alarm was not triggered during the second and third peak concentrations (on around August 20 and August 23). Similar variations were also observed in CO concentrations (Fig. S3 and Table S4).

Table 2

Summary statistics for PM_{2.5} measurements during the wildfire episodes in Portland, OR.

	Initial Installation ^a	After 1st-Calibration	After 2nd-Calibration	Without 2nd-Calibration
Time	08/02/2018 09:00 pm ~ 08/ 08/2018 15/2018 9:00 pm	08/08/2018 9:00 pm ~ 08/ 15/2018 12:00 am	08/15/2018 12:00 am ~ 09/14/2018 10:00 am	08/15/2018 12:00 am ~ 09/14/2018 10:00 am
R ²	0.90 / 0.88	0.99 / 0.99	0.97 / 0.97	0.97 / 0.97
RMSE ^b	1.61 / 1.62	4.06 / 5.256	3.85 / 3.82	4.09 / 4.83
MAE ^b	1.11 / 1.13	2.29 / 2.87	2.15 / 2.27	2.26 / 2.74
MBE ^b	-0.45 / -0.49	1.53 / 2.33	0.34 / 0.56	1.03 / 1.80

^a The results of sensor #02 was shown on the left, and the results of sensor #03 was shown on the right

^b The units of RMSE, MAE, and MBE are calculated in $\mu\text{g}/\text{m}^3$

This *in situ* calibration method – by simply deploying/co-locating a reference method by the LCAQS – illustrates an approach for optimally ensuring the accuracy of LCAQS data. If the LCAQS data were calibrated using conventional post-processing methods, this additional round of calibration would either occur later, after the wildfire event or not at all, resulting in a correction using prior calibration coefficients (depicted in Fig. 4 as “w/o 2nd Cali.”). Any data generated using previous calibrations would be less accurate, potentially impacting risk management related to air pollution levels, especially during elevated pollution episodes (Fig. S4 and S5).

This example shows that the *in situ* calibration can be more efficient and accurate than the conventional approaches. Beyond some earlier studies [56,57], how the *in situ* calibration could be carried out warrants further investigations. In an ideal situation, a hybrid LCAQS and regulatory network should be established according to the spatial homogeneity of a specific pollutant (see Section 3.1). Once a recalibration alert

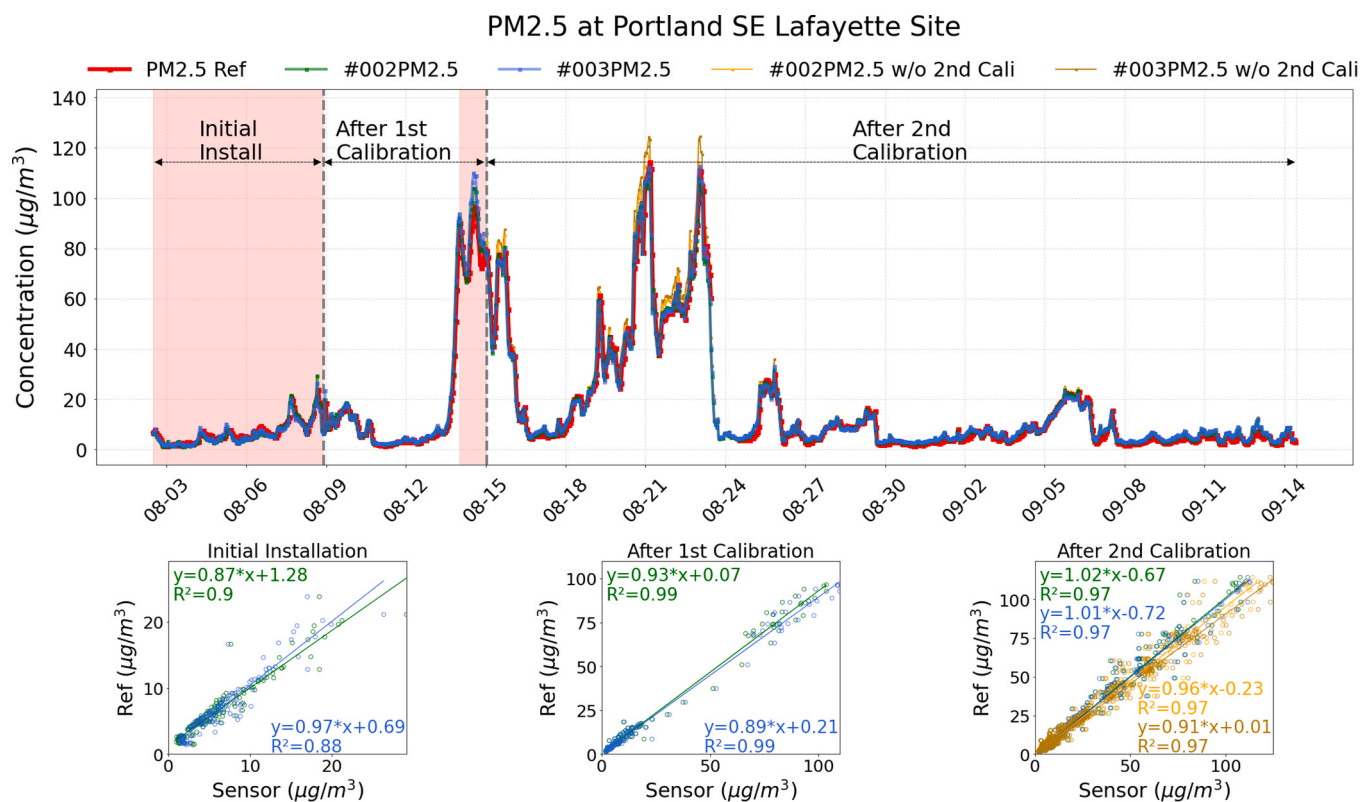


Fig. 4. Hourly data of two PM_{2.5} sensors and the reference data during the wildfire episodes in Portland from August 2 to September 14, 2018. Periods shaded in pink color indicate the calibration periods where the sensors were co-located with a reference method. During the non-shaded periods, sensors reported data based on the prior calibration results.

is triggered, *in situ* calibration should be set up in a short period of time either by the installation of a portable reference monitor next to the sensor(s) or by relocating the LCAQS to a nearby reference station. We recommend collecting at least one additional day of calibration data for machine learning, but the exact co-location time to achieve the best calibration results should be established for a particular study region.

4. Conclusions

To investigate effective LCAQS network design strategies, we analyzed three years of EPA AQS data. Our results indicated that the spatial homogeneity of air pollutants, especially for PM_{2.5}, CO, and NO₂, was case-specific and varied by geography considered. Identifying the specific pollutant of most concern in the target area prior to planning any sensor networks is essential for designing an optimal LCAQS network. To find the most sustainable method to deploy LCAQS, it is recommended that pilot studies be conducted to investigate the regional homogeneity of targeted pollutants.

Systematic bias between different FEM methods can cause significant bias in the LCAQS evaluation, illustrating the importance of specifying the type of FEM instruments selected for sensor evaluation. Combined with the data reported from SC-AQSPEC, we found PM_{2.5} sensors displayed a better fitting performance with light scattering principle reference instruments (e.g., GRIMM and T640) compared to other methods (e.g., BAM and TEOM). Sensor data during the wildfire episodes demonstrated that *in situ* machine learning calibration process enhanced the performance of LCAQS and had the promising ability to ensure the data accuracy of LCAQS during routine operations. More seasonal, non-peak pollution data is needed to further improve the *in situ* machine learning calibration, but the system's ability to adapt to heavy pollution episodes is promising. By addressing these three critical questions of LCAQS applications, our work highlights the capability of LCAQS as a promising supplement to regulatory stations for air pollutant monitoring and emphasizes the urgent need for establishing and agreeing upon "good practice" guidelines for LCAQS network design, deployment, and management.

CRedit authorship contribution statement

Yi Li: Conceptualization, Methodology, Investigation, Writing – original draft, Writing – review & editing, Visualization, Project administration, Funding acquisition. **Ziyang Yuan:** Methodology, Investigation, Formal analysis, Writing – review & editing, Visualization. **L.-W. Antony Chen:** Conceptualization, Methodology, Writing – review & editing. **Ajay Pillarisetti:** Methodology, Investigation, Writing – review & editing. **Varun Yadav:** Conceptualization, Investigation, Writing – review & editing. **Mengxian Wu:** Investigation, Formal analysis, Visualization. **Houxin Cui:** Conceptualization, Project management, Writing – review & editing. **Chuanfeng Zhao:** Conceptualization, Methodology, Writing – review & editing.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Supporting information

Supplementary data associated with this article can be found in the online version at doi:10.1016/j.snb.2021.130958.

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