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A novel calibration approach of MODIS AOD data to predict PM_{2.5} concentrations

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Abstract

Epidemiological studies investigating the human health effects of PM_{2.5} are susceptible to exposure measurement errors, a form of bias in exposure estimates, since they rely on data from a limited number of PM_{2.5} monitors within their study area. Satellite data can be used to expand spatial coverage, potentially enhancing our ability to estimate location- or subject-specific exposures to PM_{2.5}, but some have reported poor predictive power. A new methodology was developed to calibrate aerosol optical depth (AOD) data obtained from the Moderate Resolution Imaging Spectroradiometer (MODIS). Subsequently, this method was used to predict ground daily PM_{2.5} concentrations in the New England region. 2003 MODIS AOD data corresponding to the New England region were retrieved, and PM_{2.5} concentrations measured at 26 US Environmental Protection Agency (EPA) PM_{2.5} monitoring sites were used to calibrate the AOD data. A mixed effects model which allows day-to-day variability in daily PM_{2.5}-AOD relationships was used to predict location-specific PM_{2.5} levels. PM_{2.5} concentrations measured at the monitoring sites were compared to those predicted for the corresponding grid cells. Both cross-sectional and longitudinal comparisons between the observed and predicted concentrations suggested that the proposed new calibration approach renders MODIS AOD data a potentially useful predictor of PM_{2.5} concentrations. Furthermore, the estimated PM_{2.5} levels within the study domain were examined in relation to air pollution sources. Our approach made it possible to investigate the spatial patterns of PM_{2.5} concentrations within the study domain.

1 Introduction

Atmospheric aerosols originate from natural and anthropogenic emission sources. Particularly, anthropogenic aerosols are considered to have major human health implications, and numerous studies have reported associations between mortality and morbidity and particulate matter with aerodynamic diameter $\leq 2.5 \mu\text{m}$ (PM_{2.5}) (Bell et al., 2007; Dominici et al., 2006; Franklin et al., 2007; Gent et al., 2003, 2009; Schwartz et al.,

1996; Slama et al., 2007). The $PM_{2.5}$ health effect studies generally use $PM_{2.5}$ measurements from ground monitoring sites, but there are many regions with no ground $PM_{2.5}$ measurements available due to their sparse monitoring networks. This limits the ability of estimating human exposures to $PM_{2.5}$, which is likely to cause less reliable health effect assessments.

Satellite remote sensing can be used to assess $PM_{2.5}$ air quality for areas where surface $PM_{2.5}$ monitors are not available (Di Nicolantonio et al., 2009; Engel-Cox et al., 2004; Gupta and Christopher, 2008; Gupta et al., 2006; Koelemeijer et al., 2006; Liu et al., 2004; Schaap et al., 2009; van Donkelaar et al., 2010). The most applicable satellite-retrieved product for estimating $PM_{2.5}$ concentrations is aerosol optical depth (AOD), which measures the light extinction by aerosol scattering and absorption in the atmospheric column. Since the AOD reflects the integrated amount of particles in the vertical column, it has been used as an input parameter in statistical models predicting $PM_{2.5}$ levels. In addition to AOD values, several studies have also included other predictor parameters such as local meteorology and land use information (e.g., population density). As reported by previous studies, these parameters influence the relationship between AOD and ground-level $PM_{2.5}$ concentrations, thus can be used as additional predictors (Liu et al., 2005, 2007a, b, c, 2009). However, these models, developed by us and others, generally predict <60% of the variability in daily $PM_{2.5}$ concentrations (Paciorek et al., 2008). Additional time-varying parameters influence the $PM_{2.5}$ -AOD relationship, including $PM_{2.5}$ vertical and diurnal concentration profiles, PM optical properties, and others. Therefore, it is reasonable to expect that the relationship between $PM_{2.5}$ and AOD varies by day. In this paper we introduce a new approach to calibrate Moderate Resolution Imaging Spectroradiometer (MODIS) AOD data to accurately predict $PM_{2.5}$ ground concentrations.

Our method is unique because it establishes day-specific $PM_{2.5}$ -AOD relationships using a mixed effects model to fully exploit satellite data. To the best of our knowledge, no previous studies have suggested a statistical approach establishing the $PM_{2.5}$ -AOD relations on a daily basis.

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2 Methods

2.1 Ground-level $PM_{2.5}$ data

Our study region includes the States of Massachusetts (MA), Connecticut (CT), and Rhode Island (RI) in the Northeastern US. To calibrate satellite data, daily $PM_{2.5}$ concentrations measured at 26 US Environmental Protection Agency (EPA) $PM_{2.5}$ monitoring sites were used (Fig. 1). For collocated monitors, we calculated the daily averages of the $PM_{2.5}$ concentrations. Samples were collected at 15 Connecticut sites and 11 Massachusetts sites during the period 1 January through 31 December 2003. Sampling frequency differed by site including collecting samples every day, every third day, and every sixth day.

2.2 AOD retrieval

MODIS aboard the National Aeronautics and Space Administration (NASA)'s Earth Observing System (EOS) satellites, Terra and Aqua, was used to retrieve AOD (Collection 5; Level 2 aerosol product) for the year 2003. The Terra and Aqua satellites were launched in December 1999 and in May 2002, respectively. These polar-orbiting satellites, operating at an altitude of approximately 700 km, provide data every one to two days under cloud-free conditions. Their sensors scan the swath of 2330 km (cross-track) by 10 km (along-track at nadir) and gather information on particle abundance once from each satellite: approximately 10:30 a.m. and 1:30 p.m. local times for Terra and Aqua, respectively. In the Collection 5 retrieval algorithm, three different channels of 0.47, 0.66, and 2.12 μm are primarily employed for over-land retrievals. The channels of 0.47 and 0.66 μm are used to retrieve AOD values which are interpolated to report AOD values at the wavelength of 0.55 μm , and the uncertainty of the MODIS AOD is expected to be $\Delta\text{AOD} = \pm 0.05 \pm 0.15 \times \text{AOD}$ over land. Furthermore, the maximum AOD value is constrained to be 5.0, and negative AOD values down to -0.05 were retained in order to avoid bias that can occur when truncating or omitting low

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the measured and predicted mean $PM_{2.5}$ concentrations before taking the site bias into account at the New Haven site can be explained by the fact that this site is not representative of the corresponding grid cell $10 \times 10 \text{ km}^2$ area, and it indicates that the approach of controlling for the site bias in the mixed effects model is reasonable for the comparisons between the measured and predicted $PM_{2.5}$ concentrations. However, considering that AOD-derived $PM_{2.5}$ concentrations reflect the overall $PM_{2.5}$ levels in the grid cell, the unadjusted predicted $PM_{2.5}$ levels may be more representative of the average population exposures to $PM_{2.5}$.

AOD retrieval errors due to unscreened clouds could introduce positive bias. The current cloud screening algorithm in AOD retrievals (Collection 5) effectively masks clouds, but it is still possible to have AOD values affected by clouds, particularly for isolated and residual clouds (Levy et al., 2007). The comparison between MODIS AOD and the Aerosol Robotic Network (AERONET) AOD (Level 2.0; within ± 30 min of Terra measurements) in Billerica could indicate days with positive bias potentially from isolated and residual clouds in the area (correlation $r = 0.92$; slope = 1.20; intercept = -0.002 in a linear regression model between the MODIS AOD and the AERONET AOD data) (Holben et al., 1998). Consequently, the AOD values overestimated by the clouds may cause positive bias in predicted $PM_{2.5}$ concentrations. In part, $PM_{2.5}$ measurement errors might cause positive or negative bias in measured $PM_{2.5}$ levels.

The ability of the mixed effects and linear regression models to predict $PM_{2.5}$ concentrations was compared. For each model the predicted concentrations were regressed on the observed ones for each site separately (Table 4 and Fig. 3). It should be noted that the CV method produces less biased estimates than those obtained from the model fit (shown in Tables 3 and 4). The two models were compared using results from CV analyses to avoid over-fitting thus to produce more robust results. Note that the predicted $PM_{2.5}$ concentrations in the mixed effects model were not adjusted for the site bias (Table 4 and Fig. 3). The mixed effects model explained 95% of the variability in the measured $PM_{2.5}$ concentrations on average, ranged from 82% in Boston, MA (Site ID: 25-025-0027) to 100% in Bridgeport, CT (Site ID: 09-001-0010). On the

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other hand, in the linear regression model, the mean variability of the measured $PM_{2.5}$ explained by the predicted $PM_{2.5}$ was 51%, ranging from 12% in Boston, MA (Site ID: 25-025-0027) to 88% in Stamford, CT (Site ID: 09-001-2124). While the regression model yielded modest and considerably varying predictability by site, our model demonstrated consistently high predictability for most of the sites. These findings suggest that predicting $PM_{2.5}$ within a domain requires the use of daily calibrations. This explains why previous investigations have not demonstrated that AOD can be a robust predictor of $PM_{2.5}$ (Paciorek and Liu, 2009; Paciorek et al., 2008).

The predictive ability of our model was also compared to that of the regression model in terms of percent precision (% Precision) (Table 4 and Fig. 3). Note that this comparison was performed using the CV results as well. Since the R^2 does not reflect systematic differences between the measured and predicted $PM_{2.5}$ levels, the measure of precision (% Precision) is necessary to better assess model performance. In the mixed effects model, the % CV precision ranged from 8.8% ($1.08 \mu\text{g m}^{-3}$) in New Haven, CT (Site ID: 09-009-0026) to 38.6% ($4.08 \mu\text{g m}^{-3}$) in Lynn, MA (Site ID: 25-009-2006) with the mean value of 20.0% ($2.45 \mu\text{g m}^{-3}$). For the regression model the estimated mean % CV precision was 59.5% ($7.40 \mu\text{g m}^{-3}$), varying from 41.1% ($4.59 \mu\text{g m}^{-3}$) in Fall River, MA (Site ID: 25-005-1004) to 89.8% ($12.73 \mu\text{g m}^{-3}$) in Boston, MA (Site ID: 25-025-0027).

With regard to the measures of CV R^2 and precision values, our model presented considerably higher CV R^2 (0.95) and lower CV precision (20.0%, $2.45 \mu\text{g m}^{-3}$) than those estimated for the regression model (CV $R^2 = 0.51$, % CV precision = 59.5% ($7.40 \mu\text{g m}^{-3}$)). Also, the cross-sectional comparison between the measured and predicted site mean $PM_{2.5}$ concentrations was performed for both models. As shown in Fig. 4, a higher correlation coefficient ($R^2 = 0.62$; Pearson $r = 0.79$) was determined for the mixed effects model as compared to that estimated for the linear regression model ($R^2 = 0.26$; Pearson $r = 0.51$). Overall, the performance of the mixed effects model to predict surface-level $PM_{2.5}$ concentrations was superior as compared to that of the regression model. Collectively, these performance tests suggest that the mixed effects

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Table 1. PM_{2.5} concentrations (µg m⁻³) observed at the 26 EPA monitoring sites in 2003.

Site ID	City	N	Mean	SE
09-001-0010	Bridgeport, CT	97	12.2	0.8
09-001-0113	Bridgeport, CT	94	11.7	0.8
09-001-1123	Danbury, CT	101	13.0	0.9
09-001-2124	Stamford, CT	100	13.3	0.9
09-001-3005	Norwalk, CT	99	12.0	0.8
09-001-9003	Westport, CT	108	11.0	0.7
09-003-1003	E. Hartford, CT	310	11.4	0.4
09-003-1018	Hartford, CT	92	12.3	0.9
09-009-0018	New Haven, CT	307	17.0	0.5
09-009-0026	New Haven, CT	70	11.5	1.1
09-009-1123	New Haven, CT	108	13.4	0.8
09-009-2008	New Haven, CT	79	12.0	1.1
09-009-2123	Waterbury, CT	110	12.4	0.8
09-009-8003	W. Haven, CT	77	12.6	1.1
09-011-3002	Norwich, CT	79	10.7	0.7
25-005-1004	Fall River, MA	90	10.2	0.8
25-009-2006	Lynn, MA	78	10.3	1.2
25-009-5005	Haverhill, MA	87	9.0	0.7
25-013-0008	Chicopee, MA	237	9.7	0.4
25-013-0016	Springfield, MA	265	12.8	0.5
25-013-2009	Springfield, MA	75	11.3	1.0
25-023-0004	Brockton, MA	97	10.0	0.8
25-025-0027	Boston, MA	198	11.7	0.5
25-025-0042	Boston, MA	246	11.5	0.5
25-025-0043	Boston, MA	96	13.1	0.8
25-027-0020	Worcester, MA	231	11.7	0.5

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Table 2. Site bias ($\mu\text{g m}^{-3}$) estimates for 26 EPA PM_{2.5} monitoring sites.

Site ID	City	Bias ^a	p-value
09-001-0010	Bridgeport, CT	0.77	0.18
09-001-0113	Bridgeport, CT	0.57	0.28
09-001-1123	Danbury, CT	0.47	0.40
09-001-2124	Stamford, CT	1.22	0.03
09-001-3005	Norwalk, CT	1.18	0.03
09-001-9003	Westport, CT	0.24	0.68
09-003-1003	E. Hartford, CT	-0.57	0.17
09-003-1018	Hartford, CT	-0.09	0.86
09-009-0018	New Haven, CT	4.49	< .0001
09-009-0026	New Haven, CT	0.30	0.58
09-009-1123	New Haven, CT	1.35	0.006
09-009-2008	New Haven, CT	0.03	0.96
09-009-2123	Waterbury, CT	0.46	0.34
09-009-8003	W. Haven, CT	1.70	0.002
09-011-3002	Norwich, CT	-0.08	0.89
25-005-1004	Fall River, MA	-0.27	0.66
25-009-2006	Lynn, MA	-2.64	< .0001
25-009-5005	Haverhill, MA	-1.64	0.003
25-013-0008	Chicopee, MA	-1.92	< .0001
25-013-0016	Springfield, MA	-0.001	0.998
25-013-2009	Springfield, MA	-0.55	0.31
25-023-0004	Brockton, MA	-1.71	0.002
25-025-0027	Boston, MA	-1.37	0.04
25-025-0042	Boston, MA	-0.43	0.45
25-025-0043	Boston, MA	0.004	0.996
25-027-0020	Worcester, MA	-1.48	0.002

^a Bias represents the random effect estimates of the site term in the mixed effects model.

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Table 3. Mixed effects model performance by site^a.

Site ID	City	N	PM _{2.5} measured	PM _{2.5} predicted	Bias ^b	R ²	Precision ^c	% Precision ^d
09-001-0010	Bridgeport, CT	15	11.59	11.50	-0.08	1.00	0.96	8.31
09-001-0113	Bridgeport, CT	19	9.64	9.59	-0.05	0.97	1.15	11.89
09-001-1123	Danbury, CT	16	13.96	13.91	-0.05	0.98	1.85	13.29
09-001-2124	Stamford, CT	14	12.63	12.48	-0.14	0.98	1.42	11.21
09-001-3005	Norwalk, CT	18	13.49	13.38	-0.11	0.99	1.32	9.81
09-001-9003	Westport, CT	15	11.07	11.05	-0.03	0.99	1.12	10.16
09-003-1003	E. Hartford, CT	56	13.99	14.01	0.02	0.98	1.41	10.04
09-003-1018	Hartford, CT	18	8.98	8.99	0.01	0.97	0.76	8.44
09-009-0018	New Haven, CT	45	19.46	19.30	-0.16	0.97	2.17	11.17
09-009-0026	New Haven, CT	18	12.32	12.30	-0.03	0.99	0.91	7.38
09-009-1123	New Haven, CT	25	12.54	12.45	-0.09	0.99	1.01	8.02
09-009-2008	New Haven, CT	25	14.36	14.35	0.00	0.99	1.40	9.72
09-009-2123	Waterbury, CT	25	11.44	11.41	-0.03	0.99	1.07	9.38
09-009-8003	W. Haven, CT	16	17.04	16.87	-0.18	0.98	2.77	16.28
09-011-3002	Norwich, CT	14	8.21	8.22	0.01	0.97	0.81	9.83
25-005-1004	Fall River, MA	12	11.16	11.20	0.04	0.95	2.37	21.21
25-009-2006	Lynn, MA	13	10.57	10.90	0.34	0.97	2.20	20.81
25-009-5005	Haverhill, MA	17	11.44	11.60	0.16	0.98	1.47	12.88
25-013-0008	Chicopee, MA	34	9.33	9.42	0.09	0.93	2.14	22.98
25-013-0016	Springfield, MA	44	12.73	12.73	0.00	0.97	1.70	13.39
25-013-2009	Springfield, MA	18	10.30	10.35	0.05	0.98	1.30	12.59
25-023-0004	Brockton, MA	18	8.99	9.15	0.16	0.95	2.29	25.45
25-025-0027	Boston, MA	15	14.17	14.32	0.15	0.92	2.90	20.50
25-025-0042	Boston, MA	22	15.24	15.27	0.03	0.98	1.81	11.85
25-025-0043	Boston, MA	6	15.45	15.45	0.00	0.99	1.53	9.89
25-027-0020	Worcester, MA	38	10.25	10.32	0.06	0.93	1.60	15.62

^a The measured and predicted PM_{2.5} concentrations, bias, and precision are in the unit of $\mu\text{g m}^{-3}$.

^b Bias is defined as $(\text{PM}_{2.5} \text{ predicted} - \text{PM}_{2.5} \text{ measured})$.

^c Precision is estimated as the square root of the mean of the squared errors.

^d % Precision is defined as $(100 \times (\text{precision}/\text{PM}_{2.5} \text{ measured}))$.

Table 4. Comparisons of CV R^2 and % CV Precision ($\mu\text{g m}^{-3}$ for CV precision) between the measured and predicted $\text{PM}_{2.5}$ concentrations using mixed effects model and regression model^a.

Site ID	City	N	$\text{PM}_{2.5}$ measured	$\text{PM}_{2.5}$ predicted	Bias ^b	R^2	Precision ^c	% Precision ^d
Mixed effects model								
09-001-0010	Bridgeport, CT	15	11.59	10.66	-0.93	1.00	1.45	12.54
09-001-0113	Bridgeport, CT	19	9.64	8.84	-0.80	0.95	1.77	18.33
09-001-1123	Danbury, CT	16	13.96	13.43	-0.53	0.96	2.39	17.11
09-001-2124	Stamford, CT	14	12.63	11.23	-1.40	0.98	2.10	16.64
09-001-3005	Norwalk, CT	18	13.49	12.16	-1.33	0.99	2.03	15.06
09-001-9003	Westport, CT	15	11.07	10.72	-0.36	0.98	1.44	13.00
09-003-1003	E. Hartford, CT	56	13.99	14.64	0.65	0.95	2.29	16.34
09-003-1018	Hartford, CT	18	8.98	9.05	0.06	0.95	0.98	10.91
09-009-0018	New Haven, CT	45	19.46	14.56	-4.90	0.95	5.66	29.11
09-009-0026	New Haven, CT	18	12.32	12.00	-0.32	0.99	1.08	8.78
09-009-1123	New Haven, CT	25	12.54	11.01	-1.53	0.99	1.92	15.34
09-009-2008	New Haven, CT	25	14.36	14.31	-0.05	0.99	1.54	10.72
09-009-2123	Waterbury, CT	25	11.44	10.94	-0.50	0.99	1.33	11.62
09-009-8003	W. Haven, CT	16	17.04	15.09	-1.95	0.97	3.67	21.55
09-011-3002	Norwich, CT	14	8.21	8.30	0.09	0.96	1.03	12.49
25-005-1004	Fall River, MA	12	11.16	11.25	0.09	0.92	3.03	27.13
25-009-2006	Lynn, MA	13	10.57	13.77	3.20	0.96	4.08	38.58
25-009-5005	Haverhill, MA	17	11.44	13.52	2.08	0.97	2.88	25.20
25-013-0008	Chicopee, MA	34	9.33	11.55	2.22	0.90	3.43	36.78
25-013-0016	Springfield, MA	44	12.73	12.81	0.08	0.94	2.37	18.63
25-013-2009	Springfield, MA	18	10.30	10.89	0.59	0.97	1.60	15.51
25-023-0004	Brockton, MA	18	8.99	10.94	1.95	0.94	3.30	36.69
25-025-0027	Boston, MA	15	14.17	16.04	1.86	0.82	4.64	32.72
25-025-0042	Boston, MA	22	15.24	15.70	0.46	0.95	2.90	19.02
25-025-0043	Boston, MA	6	15.45	15.48	0.03	0.99	1.82	11.75
25-027-0020	Worcester, MA	38	10.25	12.10	1.84	0.87	2.94	28.66

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Table 4. Continued.

Regression model								
09-001-0010	Bridgeport, CT	15	11.59	13.52	1.93	0.40	8.14	70.29
09-001-0113	Bridgeport, CT	19	9.64	11.95	2.30	0.67	4.43	45.95
09-001-1123	Danbury, CT	16	13.96	10.26	-3.69	0.71	8.21	58.80
09-001-2124	Stamford, CT	14	12.63	9.80	-2.83	0.88	6.96	55.10
09-001-3005	Norwalk, CT	18	13.49	12.24	-1.25	0.38	8.53	63.24
09-001-9003	Westport, CT	15	11.07	12.09	1.01	0.48	5.94	53.64
09-003-1003	E. Hartford, CT	56	13.99	13.04	-0.96	0.39	7.78	55.64
09-003-1018	Hartford, CT	18	8.98	10.76	1.78	0.41	3.84	42.79
09-009-0018	New Haven, CT	45	19.46	13.47	-5.99	0.44	11.00	56.52
09-009-0026	New Haven, CT	18	12.32	13.74	1.42	0.70	6.03	48.96
09-009-1123	New Haven, CT	25	12.54	11.84	-0.70	0.62	6.74	53.73
09-009-2008	New Haven, CT	25	14.36	14.05	-0.31	0.66	8.18	57.00
09-009-2123	Waterbury, CT	25	11.44	10.16	-1.28	0.63	5.75	50.25
09-009-8003	W. Haven, CT	16	17.04	13.28	-3.76	0.58	11.57	67.90
09-011-3002	Norwich, CT	14	8.21	9.32	1.11	0.43	4.04	49.25
25-005-1004	Fall River, MA	12	11.16	12.46	1.31	0.79	4.59	41.10
25-009-2006	Lynn, MA	13	10.57	13.80	3.23	0.72	8.73	82.56
25-009-5005	Haverhill, MA	17	11.44	12.48	1.04	0.73	6.36	55.61
25-013-0008	Chicopee, MA	34	9.33	10.19	0.86	0.25	6.19	66.39
25-013-0016	Springfield, MA	44	12.73	11.44	-1.28	0.30	8.13	63.86
25-013-2009	Springfield, MA	18	10.30	11.66	1.36	0.36	6.24	60.62
25-023-0004	Brockton, MA	18	8.99	11.02	2.03	0.44	5.76	64.03
25-025-0027	Boston, MA	15	14.17	21.08	6.90	0.12	12.73	89.83
25-025-0042	Boston, MA	22	15.24	18.24	3.00	0.40	10.25	67.24
25-025-0043	Boston, MA	6	15.45	19.44	3.99	0.68	9.54	61.74
25-027-0020	Worcester, MA	38	10.25	12.54	2.28	0.17	6.63	64.69

^a The measured and predicted $\text{PM}_{2.5}$ concentrations, bias, and precision are in the unit of $\mu\text{g m}^{-3}$.

^b Bias is defined as $(\text{PM}_{2.5} \text{ predicted} - \text{PM}_{2.5} \text{ measured})$.

^c Precision is estimated as the square root of the mean of the squared errors.

^d % Precision is defined as $(100 \times (\text{precision}/\text{PM}_{2.5} \text{ measured}))$.

9790

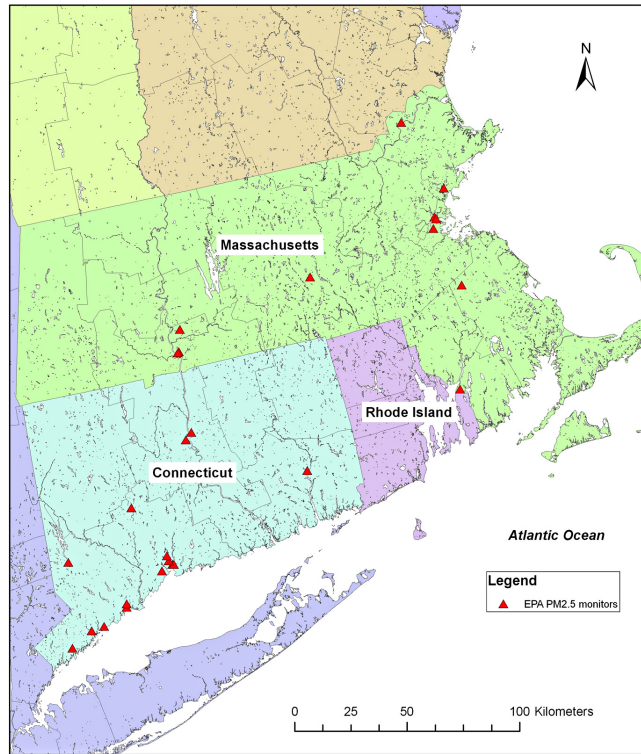


Fig. 1. PM_{2.5} monitoring site locations in 2003.

9791

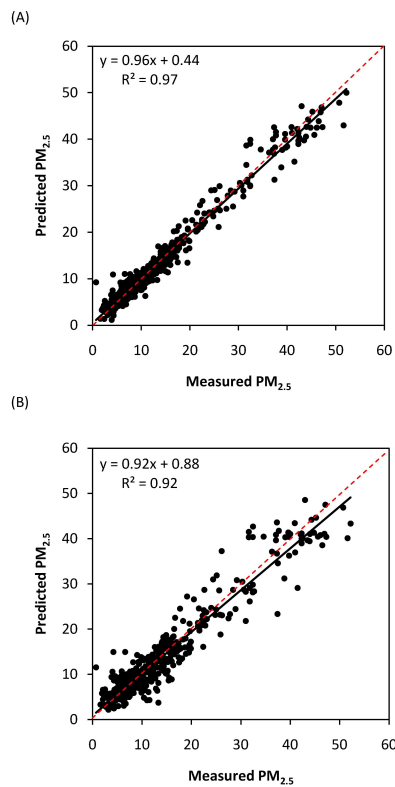


Fig. 2. Mixed effects model performance assessed by 576 measured and predicted daily PM_{2.5} concentrations ($\mu\text{g m}^{-3}$) from: **(A)** mixed effects model and **(B)** CV mixed effects model. The solid line represents the regression line, and the dashed line displays the 1:1 line.

9792

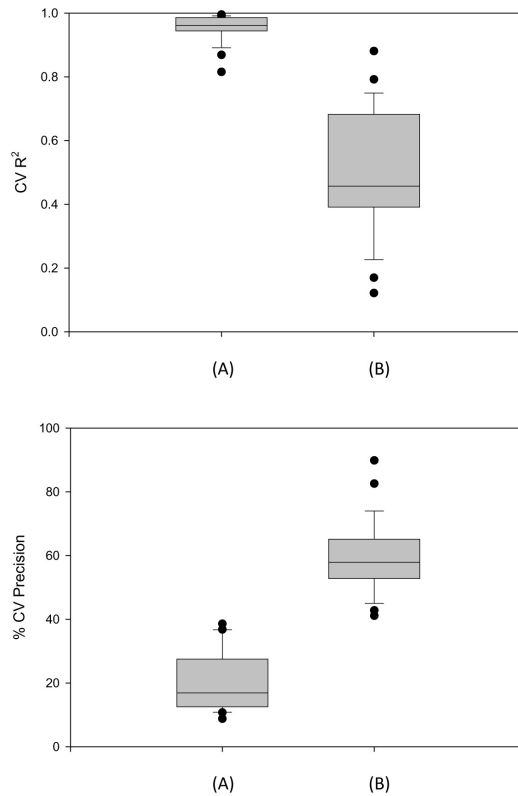


Fig. 3. Cross-validation correlation coefficients and % Precision between the measured and predicted PM_{2.5} concentrations for the: **(A)** mixed effects model and **(B)** regression model.

9793

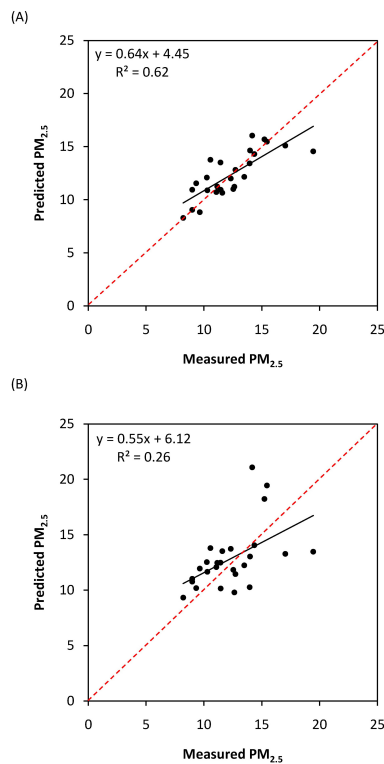


Fig. 4. Cross-sectional comparisons between the measured and predicted site mean PM_{2.5} concentrations ($\mu\text{g m}^{-3}$) for the: **(A)** mixed effects model and **(B)** regression model (both from CV analyses). The solid line represents the regression line, and the dashed line displays the 1:1 line.

9794

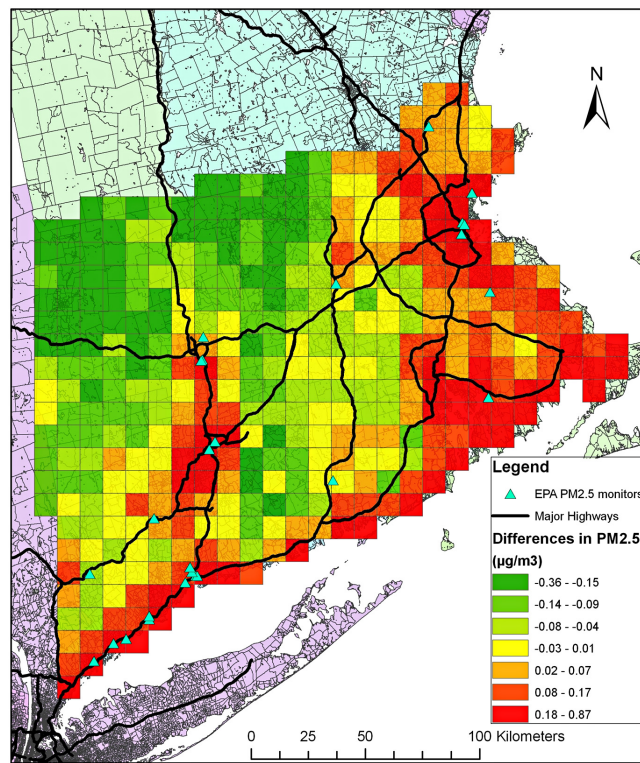


Fig. 5. Spatial variability in PM_{2.5} levels in the study region. PM_{2.5} levels are expressed as differences between grid-specific predicted and regional PM_{2.5} concentrations (µg m⁻³).