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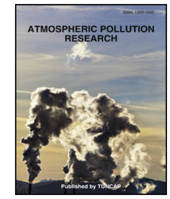

Applying machine learning methods in managing urban concentrations of traffic-related particulate matter (PM_{10} and $PM_{2.5}$)

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ABSTRACT

This study presents a new method for evaluating the effectiveness of roadside PM_{10} and $PM_{2.5}$ reduction scenarios using Machine Learning (ML) based models. The ML methods include Artificial Neural Networks (ANN), Boosted Regression Trees (BRT) and Support Vector Machines (SVM). Traffic, meteorological and pollutant data collected at nineteen Air Quality Monitoring (AQM) sites in London for a period between 2007 and 2012 was used. The ML models performed very well in predicting the concentrations of PM_{10} and $PM_{2.5}$ with around 95% of their predictions falling within the factor of two of the observed concentrations at the roadsides. The prediction errors observed were very small as indicated by the average normalised mean gross errors of 0.2. Also, the predictions of the models correlated well with the observed concentrations as shown by the average values of R (0.8) and index of agreement (0.74). Additionally, when some PM_{10} and $PM_{2.5}$ reduction scenarios were modelled, the ML models predicted various degree of reductions in the roadside concentrations. In conclusion, well trained ANN and BRT models can be successfully applied in predictions of roadside PM_{10} and $PM_{2.5}$ concentrations. Moreover, they can be applied in measuring the effectiveness of roadside particle reduction scenarios.

1. Introduction

Urban air pollution is increasingly becoming the major environmental concern in cities around the world. The growth of population within major cities has resulted in an unprecedented increase in activities and higher demands for energy and transportation. These factors contribute significantly to urban air pollution emanating from often congested major road networks. Urban air pollution can be effectively managed through careful planning and execution of Urban Air Quality Management (UAQM). The key components of UAQM consist of a clear definition of objectives and standards, well-designed air quality monitoring network and reliable air quality modelling. These components help in the design of air quality control strategies and in measuring their effectiveness. Air quality modelling is an important aspect of the UAQM as it helps in taking a decision on the main issues relating to the budget for the UAQM and predicting the likely effects of potential control strategies.

Machine Learning (ML) techniques have been used in air quality modelling in the last two decades (Yi and Prybutok, 1996; Gardner and Dorling, 1998). A search for more viable models than the operational air quality models leads to many studies on the use of various ML methods in air quality modelling. Operational air quality models such as ADMS-Roads (Mchugh et al., 1997) and OSPM (Berkowicz, 2000) require understanding of the interactions between the air quality variables and meteorological conditions. Most of the operational models are deterministic and are limited in so many aspects. For example, the natural phenomenon involved are difficult to characterise accurately. Also, the use of default parameters and the lack of real observations with the same spatial resolution with which to compare the model outputs are among the limitations of the operational models (National Research Council, 2007; Chave and Levin, 2003). In addition, most of the operational air quality models are based on steady-state Gaussian plume models which are limited by the assumptions regarding changes of wind and source emissions over time and do not include the detailed chemistry of particle pollutants (Pelliccioni and Tirabassi, 2006; Lagzi et al., 2013). Other sources of uncertainty in the operational models are the inherent uncertainty associated with data required to run these models. Emission rates estimated from emissions models are an excellent example of the data needed to run the models, and in most cases, they accommodate up to ± 50% uncertainties (Debry and Mallet, 2014). Also, computational time and effort are part of the constraints that lead to the simplification of operational models.

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In contrast, machine learning methods such as Artificial Neural Networks (ANN), Boosted Regression Trees (BRT) and Support Vector Machines (SVM) can build air quality models with comparable or better accuracy. This performance can be achieved at a lower computational cost and with no assumptions on the atmospheric processes involved (Gardner and Dorling, 2000). Machine learning algorithms can handle complex and nonlinear relationships that exist between air quality variables (Esplin, 1995) and produce models that perform well in predicting unseen data (Elangasinghe et al., 2014b; Balsamà et al., 2014). ANN methods have been used in many air quality studies (Taspinar, 2015; Ragosta et al., 2015; Elangasinghe et al., 2014a) involving prediction and forecasting of air pollutants ranging from the current hour to several days in advance (Russo et al., 2013, De Gennaro et al., 2013). Many studies involving ANN often use cross-validation or evolutionary algorithms such as Genetic algorithm and particle swarm optimisation methods to derive an optimum architecture for the ANN models (Ding et al., 2011a, 2011b; He et al., 2014). Also, some air quality studies often combined ANN with feature selection methods such as PCA (Taspinar, 2015; Ragosta et al., 2015), stepwise regression (Russo et al., 2013; Lima et al., 2013), and cluster analysis (Elangasinghe et al., 2014b). Suleiman et al. (2016b) combined elastic-net regression with ANN and produced models for prediction of roadside particles with higher prediction accuracy and fewer predictor variables than standalone ANN models.

This paper presents a new method for evaluating the effectiveness of roadside PM_{10} and $PM_{2.5}$ reduction scenarios using ML based air quality models (ANN, BRT and SVM). The paper applied the Meteorological, Pollution and Traffic data collected from nineteen monitoring sites in London to train the ML models for the prediction of particle concentrations at the sites. The models were also applied to predict the likely effects of a hypothetical air quality management scenario on the concentrations.

2. Method

2.1. Air quality monitoring (AQM) sites

The AQM sites for this study were selected from the London Air Quality monitoring sites categorised as strategic by Moorcroft and Marner (2011). The strategic sites include the sites that are being used as Average Exposure Indicator Reference Sites for $PM_{2.5}$ and Low Emission Zone (LEZ) evaluation sites. They are also part of the UK Automatic Urban and Rural Network (AURN). The sites are mostly maintained by the London boroughs, Department for Environment, Food and Rural Affairs (DEFRA), and Transport for London (TfL). Additional criteria used in selecting these sites are the data availability and the type of the site. First, roadside and kerb sites with available data were chosen and either an urban or suburban site located upwind of the roadside or kerbside sites were used as their background sites.

Fig. 1 shows the distribution of the AQM sites across London and the average PM_{10} concentrations at the sites. The selected AQM sites consists of two kerbside, ten roadside, four urban background, and three suburban sites. The kerbside and roadside sites are located within 1 and 10 m from the major roads. Some of the sites (i.e. HK6, IS2, KC5, and MY1) are placed in street canyons while GR5, GR8, KC2, CR4 and CD3 sites are located near junctions. Only BT4 and GR8 sites are situated in an open area (see Table 1). The BL0, CR3, CT3, GR4, IS6 and KC1 sites are either urban or rural background monitoring sites which are mostly located in areas where there is less influence of local pollution sources. Among these sites, PM_{10} data was collected from fourteen sites while $PM_{2.5}$ data was collected from 6 sites.

2.2. Data

The data being monitored at the AQM sites include both particles and gaseous pollutants (PM_{10}, $PM_{2.5}$, NOx, NO_2, NO, SO_2, CO, and O_3), traffic volume and speeds. Others are meteorological variables wind speeds, wind direction, solar radiation, relative humidity and ambient temperature. The instruments used for the monitoring of $PM_{2.5}$ and PM_{10} at most of the sites include two similar Tapered Element Oscillating Microbalances (TEOM) Model 1400AB with different sampling heads design, filter dynamics measurement system (FDMS) and β-attenuation analysers (Aurelie and Harrison, 2005).

For this study, Traffic, Pollution and Meteorological data are required at each monitoring unit to develop the ML models. However, due to unavailability of a reliable meteorological data at the stations, data monitored at Heathrow Airport Weather Station including wind speeds, wind direction, solar radiation, relative humidity and ambient temperature was used. It was assumed that data from the Heathrow Airport gives a reasonable overview of the general meteorological conditions in London (Manning et al., 2000). The hourly pollutant data for the period between 2007 and 2012 was obtained through the London Air Archives (London Air, 2013) and UK Air Quality Archive (UK-AIR, 2013). While the meteorological data for the same period was collected from BADC data services (MIDAS Land Surface, 2013). The Continuous traffic data in London for the same period available for this study was only for MY1, HK6, BT4 and KC2 sites, therefore, at the remaining sites an estimate of the traffic was provided based on the manual count data compiled by the Department for Transport every year at some traffic count points on road links across the UK (DFT, 2014). The data collected from these sources was used for the development of the ML models.

As shown in Table 1, the average hourly traffic volume at TH4, GR8 BT4, MY1 sites was between 3327 veh/hr, and 7000 veh/hr. The average mean PM_{10} concentrations at all the sites were between 21.11μg/m^3 at KC1 and 43.25 μg/m^3 at MY1 and in most of the sites the values fell under the EU limit value of 40 μg/m^3 annual mean. The 95th percentile of the PM_{10} concentrations at the sites ranged from 49.0 μg/m^3 at BL0 to 73.8 μg/m^3 at GR8. The sites with high traffic volume were observed to have high concentrations of the particle concentrations as shown in Fig. 1. The percentages of missing data in all the sites selected were less than 10% except at KC2 where the missing data was up to 19%. The average $PM_{2.5}$ concentrations at the sites were also below the EU target value of 25 μg/m^3 annual mean. It ranged between 14μg/m^3 and 18 μg/m^3 at the five of the six roadside sites while it was 22.4 μg/m^3 at MY1. The 95th percentiles of the $PM_{2.5}$ concentrations range from 25.10 μg/m^3 at HK6 to 47 μg/m^3 at MY1. The percentages of $PM_{2.5}$ missing data at five sites were less than 10% while it was up to 18% at MY1.

The average wind speed measured at Heathrow airport between 2007 and 2012 was 2.0 m/s and the 95th percentiles, and the maximum wind speeds were 9.6 m/s and 4.2 m/s respectively (see Fig. 2). In London, the dominant winds were from the Southwest and West directions. These directions govern the location of the air quality monitoring sites. For the sites located in street Canyons, the effect of cross-Canyon vortex are caused by the prevailing wind which makes the flow circulate within the street canyon and deliver most of the pollutants to the leeward side of the street canyon (Tomlin et al., 2009), hence the location of the monitoring site. The temperature fluctuated between −6.4 in the winter and reached up to 35 °C in summer while the average temperature was 12 °C as shown in Fig. 2. More detail analysis of the data used in this study can be found in (Suleiman et al., 2016a; Suleiman, 2016).

2.3. Machine learning methods selected for the study

Machine Learning (ML) systems are sets of algorithms seeking to perform a task based on the set of training examples presented to them in the training data with limited human interaction. A typical ML process involved data representation, evaluation, and optimisation with the main goal of achieving generalisation of the unseen data. The focus of this study is the use of three supervised ML methods in air quality modelling. The methods used include Artificial Neural Networks

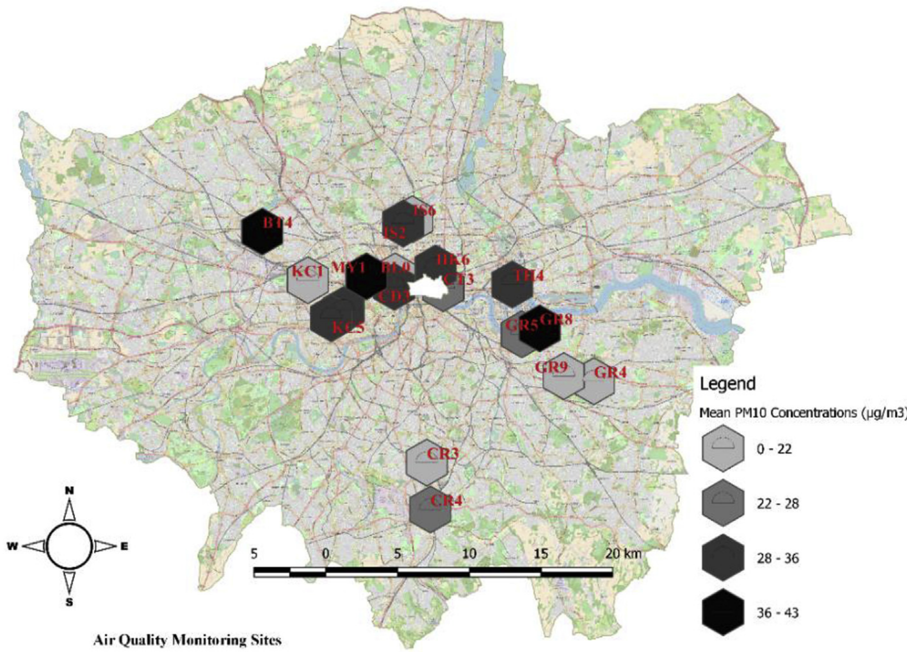


Fig. 1. Air quality monitoring sites.

(ANN), Boosted Regression Trees (BRT) and Support Vector Machines (SVM). Detailed descriptions of the ANN and BRT methods implemented in this study can be found in (Suleiman et al., 2016b) and the SVM method is described in (Chunming et al., 2010; Cherkassky and Ma, 2004; Singh et al., 2013).

2.4. Machine learning modelling

The ML modelling process adopted for this study involves five stages: data preparation, feature selection, model training, model testing and model evaluation. Each of these stages have been applied for the development of ANN, BRT and SVM based PM_{10} and $PM_{2.5}$ prediction models using R statistical software (R Developent Core Team, 2015).

2.4.1. Data preparation

The predictor variables selected for the ML modelling comprises background PM_{10} and $PM_{2.5}$, background and roadside NOx, NO_2, SO_2 and CO. PM_{10} and $PM_{2.5}$ emission rates of the traffic composition (i.e. petrol cars, diesel cars, taxi, LGV, Rigid HGV, articulated HGV, Bus and Coach and motorcycle) constitutes the traffic variables in the input space. The remaining variables are meteorological variables including Rainfall, Relative humidity, solar radiation, Temperature, Barometric Pressure, Wind Speed and Wind directions. Roadside PM_{10} and $PM_{2.5}$ are the target variables. Prior to the model training missing data were imputed using Multiple Imputations by Chained Equation (MICE) (Van Buuren, 2007, Buuren and Groothuis-Oudshoorn, 2011). The effect of the imputation on the data and the accuracy of the models was investigated. Details of the data imputation validation can be found in (Suleiman, 2016).

2.4.2. Feature selection

Principal Component Analysis (PCA) was used to pre-process the predictor variables data for the ANN models. PCA derives uncorrelated variables (i.e. PCs) that reduce the dimensionality of the input space which will enhance the performance of the ANN models to be developed. The first PCs that explained 99% of the variance in the data were selected as the model's inputs. For the BRT and SVM all the variables were used. The BRT algorithms have inbuilt mechanisms for feature selection while SVM algorithms are uses regularisation (e.g. ridge regression) to enhance the performance of the models which is independent of the dimensionality of the input space.

2.4.3. ML model training and testing

Prior to the training of the ML models, the data prepared for the modelling was divided into eighty percent for training and twenty percent for testing. Subsequently, the *train* function in caret package of R software was used to determine the optimum model parameters of all the ML models considered. The function uses a user defined resampling method (e.g. repeated k – fold cross – validation), modelling method (e.g. ANN, BRT or SVM) and its corresponding parameters (e.g. number of hidden neurons and decay values for ANN) to fit several models over the specified range of the model parameters. The range of the parameters to be used is normally determined using trial and error. The resampling method specified (e.g. repeated k – fold cross – validation) is used to hold back a sample and fit the model on the remainder of the samples. The held-out samples would then be used to evaluate the performance of the trained models. This procedure is repeated until all the samples have been used for fitting the model and as holdout samples. The optimal model parameters would then be determined based on the performance of the models built. The final models would then be fitted to all the training data set using the optimal parameters (Kuhn, 2008). A repeated version of the k-fold cross-validation was adopted in this study where $k = 10$ was used and repeated five times. The trained models were then tested for the prediction of roadside PM_{10} and $PM_{2.5}$ concentrations using the test data set. The selection of the predictor variables and the model parameters were carried out for one representative site (MY1) which is in central London. Thereafter, the same combination of input variables at each site and parameters selected for each method, were used to train and test one model for each monitoring site.

2.4.4. ML model evaluation

The performance of the models was evaluated using various functions including fraction of prediction within the factor of two of the observed concentrations (FAC2), Normalised Mean Bias (NMB), and Normalised Mean Gross Error (NMGE). Others include Root Mean Squared Error (RMSE), coefficient of correlation (R), Coefficient of

Table 1
Properties of the London monitoring sites.

Site name	Site code	Site type	Traffic Volume (veh/hr)	Available PM_{10} (%)	Mean PM_{10} (μg/m^3)	Max PM_{10} (μg/m^3)	95 Percentile PM_{10} (μg/m^3)	Available $PM_{2.5}$ (%)	Mean $PM_{2.5}$ (μg/m^3)	Max. $PM_{2.5}$ (μg/m^3)	95 Percentile $PM_{2.5}$ (μg/m^3)
Camden - Bloomsbury	BL0	Urban background		92.1	21.76	376.30	49.00	93.4	16.59	132.00	40.00
Brent - Ikea	BT4	Roadside	4389	90.4	43.25	316.00	69.60	91.4	14.60	103.40	29.90
Bexley - Thamesmead	BX3	Suburban		–				99.2	9.450	300.20	20.20
Camden - Shaftesbury Avenue	CD3	Roadside	1700	91.4	34.00	285.90	59.30				
Croydon - Thornton Heath	CR3	Suburban		91.0	21.13	452.60	45.90				
Croydon - George Street	CR4	Roadside	2500	95.0	25.00	468.40	52.30				
City of London - Sir John Cass School	CT3	Background		91.5	27.51	827.60	54.60				
Greenwich - Eltham	GR4	Suburban		99.6	21.91	252.50	47.60	89.3	15.88	241.00	37.00
Greenwich - Trafalgar Road	GR5	Roadside	1500	99.6	23.37	356.45	49.70				
Greenwich - Woolwich Flyover	GR8	Roadside	7000	97.3	40.00	527.80	73.80	98.2	16.90	375.50	32.00
Greenwich - Westhorne Avenue	GR9	Roadside	2700	–	22.80	413.10	55.30	91.1	16.74	371.40	42.90
Hackney - Old Street	HK6	Roadside	2500	94.1	31.83	303.50	56.60	95.5	16.62	206.20	25.10
Islington - Holloway Road	IS2	Roadside	2000	98.6	30.73	510.2	54.70				
Islington - Arsenal	IS6	Urban background		97.5	22.40	377.80	50.80				
Kensington and Chelsea - North Ken	KC1	Urban background		96.7	21.11	229.60	46.60	92.4	14.68	202.00	39.00
Kensington and Chelsea-Cromwell Road	KC2	Roadside	2800	81.4	33.71	445.50	54.90				38.90
Kensington and Chelsea-Earls Court Rd	KC5	Kerbside	1600	98.9	35.83	182.50	66.60				
Westminster - Marylebone Road	MY1	Kerbside	3327	97.5	43.25	422.80	70.70	82.4	21.68	135.00	47.00
Tower Hamlets - Blackwall	TH4	Roadside	6000					96.0	18.00	416.80	42.90

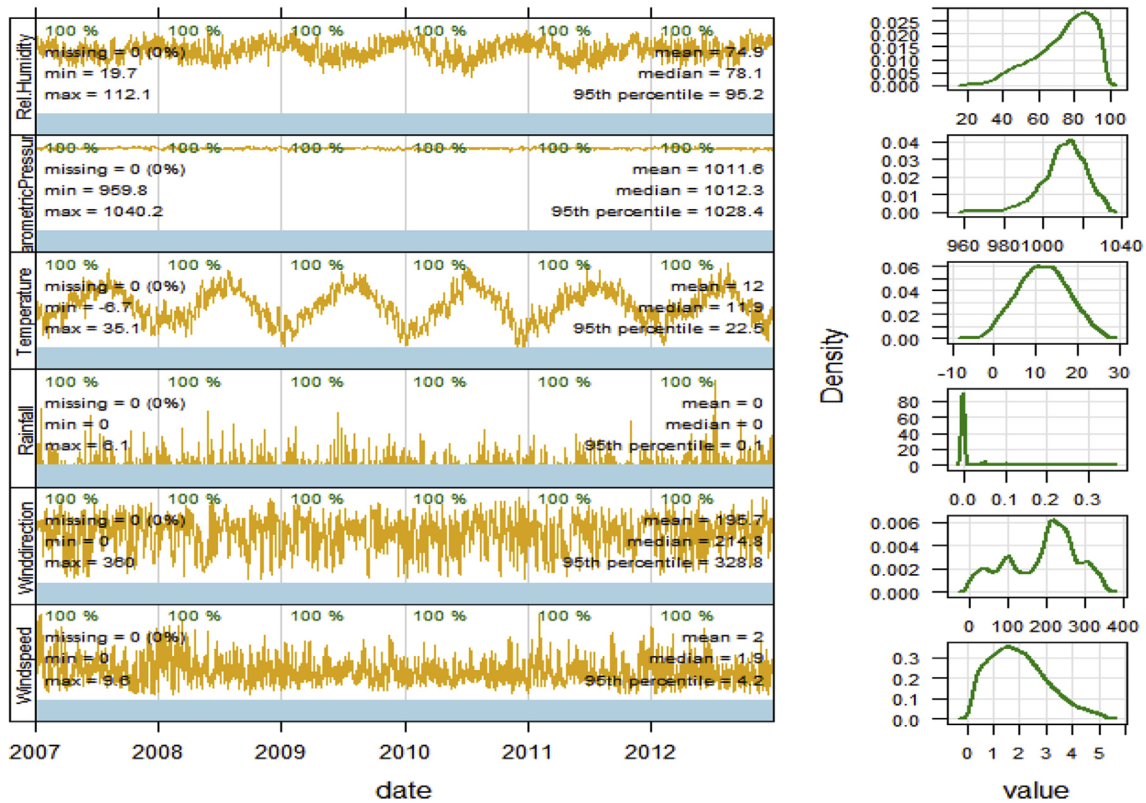


Fig. 2. Summary of the meteorological data. Note: in Fig. 2, the blue and red colours on the rectangular bar at the bottom of the plots indicate the availability and non-availability of the data respectively. The percentage of the data captured for every year is written in green on the upper part of each year data plot. The minimum, maximum, number and percent of missing data, mean, median and the 95th percentile for each variable plotted are shown in black. The panel to the right of the time series plots is the density plots indicating the distribution of the data over the selected periods.

Efficiency (COE) and Index of Agreement (IOA). The models were also evaluated based on their accurate prediction of annual statistics of the particle concentrations.

2.5. EUROIV/VI air quality management scenario

The main contribution of this paper is to investigate the use of the ML methods in evaluating the effectiveness of air quality management options involving reduction PM_{10} and $PM_{2.5}$ concentrations. To achieve this goal, a hypothetical air quality management scenario called EUROIV/VI scenario was conceptualised to verify the use of the ML models in real life applications. The EUROIV/VI scenario assumed that only EUROIV/4 petrol and EUROVI/6 diesel vehicle standards will be permitted to drive on the roads in the study area in 2011 and 2015. The emission standard restriction proposed in the scenario was implemented through LAQM Emission Factor Toolkit (EFT) version 6.0.1 (DEFRA, 2015). The EFT requires vehicle counts (veh/hr), average speed (km/hr), link length, road type, road name, projection of vehicle composition and Euro traffic composition (Euro1, Euro2, Euro III, Euro6 etc.) as inputs. The fleet composition data in London for motorways, central, inner and outer areas was used in the EFT to estimate the emission rates from the total traffic for PM_{10} and $PM_{2.5}$ including PM_{10} and $PM_{2.5}$ from tyre, brake wear and road abrasion emission sources.

As stated in section 2.4.1, the traffic emissions were selected as part of the input variables for the ML models. The use of the emission rate as part of the input data for the ML models is expected to provide a channel through which the response of the models to the changes in the emissions can be investigated. If the response of the models is positive, then they could be used as management tools for measuring traffic-related air quality control scenarios. Otherwise, they could only be used for prediction of the actual concentrations. Therefore, the difference between the emission rates estimated with and without the scenario was obtained. The average difference between the two emission rates was then subtracted from the hourly emission rates used to estimate the traffic emissions in the input data to reflect the changes due to the scenario assumptions. It is important to note that the scenario did not forecast any changes in the number of vehicles entering the study area for simplicity. Consequently, the emission rates were estimated based on the premise that all the vehicles have met the minimum standard imposed. After the traffic emissions were estimated based on the scenario, the ML models were used to predict the PM_{10} concentrations in 2011 and in 2015. For the $PM_{2.5}$, the models were tested for 2012 and 2015 due to data availability.

3. Results and discussion

3.1. Predictor variable importance

The most important variables for the ANN models were determined using PCA. The results show that the first two PCs contributed about 49% and 90% of the total variation in the input data for the PM_{10} and $PM_{2.5}$ models respectively (see Table 2).

The results from the PCA show that vehicle emissions are the most influential variables in PC1 and carry about 35 and 77% proportion of variance in the data for the PM_{10} and $PM_{2.5}$ ANN models training respectively. The next most important variables are the roadside and background NO_2 and NOx, followed by temperature, wind directions and temporal variables respectively. The contribution of the variables in the case of PM_{10} models is more distributed across the PCs than in the case of $PM_{2.5}$ models. The first PCs captured the most important positive relationship between the traffic variables and the roadside

Table 2
Principal component analysis.

Principal Components (PCs)	Proportion of Variance (PM_{10}) %	Important Variables (PM_{10})	Proportion of Variance ($PM_{2.5}$) %	Important Variables ($PM_{2.5}$)
PC1	35.23	Vehicle Emissions (g/km)	77.38	Year and Vehicle Emissions (g/km)
PC2	13.69	Background (NO_2/NO_x) (μg/m^3)	13.21	Background (NO_2/NO_x) (μg/m^3)
PC3	9.92	Background and Roadside (NO_2/NO_x) (μg/m^3)	7.72	Background and Road (NO_2/NO_x) (μg/m^3)
PC4	6.18	Temperature (^{0}C)	0.63	Year, Vehicle Emissions (Rigid/Articulated/ motorcycles) (g/km)
PC5	4.15	Month of the year	0.32	Temperature (^{0}C)
PC6	4.10	Background SO2 (μg/m^3)	0.19	Rainfall (mm)
PC7	3.72	Wind Direction (^{0}N)	0.16	Day of the month
PC8	3.51	Day of the month	0.12	Wind Direction (^{0}N)
PC9	3.34	Rainfall (mm)	0.12	Background SO_2 (μg/m^3)
PC10	2.87	Year	0.06	Month of the year
PC11	2.38	Hour of the day	0.04	Hour of the day
PC12	2.04	Barometric pressure (mBar)	0.02	Diesel car emission (g/km)
PC13	1.96	Wind speed (m/s)	0.02	Motorcycle emission (g/km)
PC14	1.76	Background PM_{10} (μg/m^3)	0.01	Background $PM_{2.5}$ (μg/m^3)
PC15	1.37	Background CO (μg/m^3)	0.00	Wind speed (m/s)
PC16	0.96	Solar Radiation (W/m^2)	0.00	Background CO (μg/m^3)
PC17	0.86	Relative Humidity (%)	0.00	Relative Humidity (%)
PC18	0.60	Roadside NO2, NOx and CO (μg/m^3)	0.00	Background (NO_2/SO_2) (μg/m^3)
PC19	0.45	Background NOx/NO2 and Roadside NOx and CO (μg/m^3)	0.00	Background (NO_2/NO_x) Roadside (NOx/CO) (μg/m^3)
	99.06		100	

pollutants. Also, the second PCs show the inverse relationships between the temperature and wind speeds on one hand, and roadside and background pollutants on the other hand. This is an indication of rising pollution levels during cold temperature which might be as result of high residential heating and condensation of volatile compounds. The pollution levels could also decrease when urban ventilation increases. The information gained from the PCA suggest that accurate data on traffic, background/roadside pollutant and meteorological variables could help in developing ML models that can predict the levels of roadside particles with reasonable accuracy. Moreover, controlling gaseous pollutants such as NOx might contribute in reducing the particle concentrations or it can serve as a reasonable proxy for the particle concentrations.

Unlike the ANN method, the BRT, identified roadside NOx, NO_2, CO and background particle concentrations as the most contributing predictor variables to the performance of the models. In addition, the contribution of the remaining variables was nearly the same and very small compared to those mentioned.

3.2. ANN, BRT and SVM model parameters

The model parameters for the ANN method are the number of hidden neurons, and weight decay. Optimum weight decay values were selected from 0, 0.001, 0.01, 0.1, 0.2, 0.5, 0.7, 0.8, 0.9, and 1, and the optimum number of hidden neurons was searched between 1 and 50. The performance of the models with different weight decay values (> 0) was observed to vary only little while higher number of hidden neurons leads to marginally better models than those with small number. The final models selected for the PM_{10} and $PM_{2.5}$ predictions, were the models trained with 49 hidden neurons and the weight decay values of 0.8 and 1.0 respectively. The number of the Principal Components (PCs) which explained 99% of the variance in the data were found to be 19 for both PM_{10} and $PM_{2.5}$ models.

The optimum BRT parameters for each pollutant were searched between five different learning rates (i.e. 0.001, 0.01, 0.05, 0.1, and 0.5), the number of trees from 1 to 10,000, tree complexities from 1 to 10 and a fixed bag fraction of 0.5. The learning rate (lr = 0.1), tree complexities (d= 5) and number of trees (1000) gave the models with the best performance for both PM_{10} and $PM_{2.5}$ predictions.

SVM parameters determined during the training were the type of kernel, the cost and sigma parameters. Therefore, linear and radial basis kernels were selected for the training. The algorithm was tuned to 15 cost values between 0.25 and 4096 on a log scale while the sigma values were empirically determined using a formula in the R statistical software package (Meyer et al., 2015). The SVM models with the combination of the cost and sigma values that yields best-performing models were selected as the final models. The optimum values of cost and sigma values were found to be 16 and 0.03 for the PM_{10} model and 8 and 0.03 for the $PM_{2.5}$ model respectively. The performance of the ML methods during parameter selection is shown in Table 3. The results show that BRT and SVM models for PM_{10} predictions performed slightly better than the ANN models as indicated by the smaller RMSE values (7.99 and 7.72).

However, for the $PM_{2.5}$ prediction models, all the three methods performed similarly with BRT performing slightly better than the ANN and SVM.

3.3. Test performance of the ML models in predicting PM_{10} and $PM_{2.5}$ concentrations

The ANN and BRT models performed similarly during testing as indicated by most of the performance statistics shown in Table 4. However, the SVM model performed slightly worse than the ANN and BRT methods. The predictions of the models are much better than what could be explained by the mean of the observed concentrations measured by the COE values (> 0). The *IOA* values ranging between 0.71 and 0.78, show that the predictions have good agreement with the PM_{10}

Table 3
Training performance of the machine learning models.

Row Labels	RMSE (μg/m^3)
PM_{10}	
ANN	9.08
BRT	7.99
SVM	7.72
PM2.5	
ANN	4.53
BRT	4.24
SVM	4.61

Table 4
Test performance of the ML models.

Model	Performance Statistics	Lower – Upper PM_{10}	Average for all sites	Lower – Upper $PM_{2.5}$	Average for all sites
Pollutant		PM_{10}		$PM_{2.5}$	
ANN	FAC2	0.84–0.99	0.97	0.93–0.98	0.95
BRT	FAC2	0.82–1.00	0.97	0.94–0.99	0.97
SVM	FAC2	0.84–0.99	0.95	0.91–0.97	0.95
ANN	NMB	−0.07–0.11	0.00	0.02–0.12	0.03
BRT	NMB	−0.03–0.15	0.02	−0.01–0.04	0.02
SVM	NMB	−0.26–0.04	−0.13	−0.06–0.01	−0.01
ANN	R	0.45–0.95	0.81	0.82–0.95	0.87
BRT	R	0.43–0.95	0.81	0.83–0.95	0.88
SVM	R	0.43–0.95	0.79	0.81–0.95	0.87
ANN	COE	0.31–0.71	0.53	0.37–0.70	0.54
BRT	COE	0.35–0.73	0.56	0.45–0.68	0.56
SVM	COE	0.33–0.70	0.45	0.44–0.70	0.54
ANN	RMSE	4.69–19.17	10.12	4.15–6.30	4.80
BRT	RMSE	4.48–20.98	10.05	3.47–6.33	4.67
SVM	RMSE	4.91–19.17	11.44	3.50–6.74	4.84
ANN	NMGE	0.13–0.38	0.20	0.17–0.26	0.20
BRT	NMGE	0.14–0.44	0.19	0.16–0.22	0.19
SVM	NMGE	0.13–0.37	0.22	0.17–0.24	0.20
ANN	IOA	0.58–0.86	0.75	0.69–0.85	0.77
BRT	IOA	0.52–0.86	0.75	0.73–0.86	0.78
SVM	IOA	0.59–0.85	0.71	0.72–0.85	0.77

Note: Table 4 show that the performance in terms of FAC2, NMB, NMGE, RMSE, R, COE and IOA values. The first and the second columns display the names of the models and the performance statistics respectively. The rest of the columns show the upper, lower and average values of the performance statistics for all the AQM sites. The third and the fourth represent the statistics for PM_{10} concentrations while the fifth and the sixth columns represent the statistics for $PM_{2.5}$ concentrations.

and $PM_{2.5}$ observations.

Also, about 95% of the model predictions fall within the factor of two of the observations as indicated by FAC2 values. The bias values of the SVM models for PM_{10} predictions are predominantly negative which signifies under prediction. It also overestimated the $PM_{2.5}$ concentrations at all the sites except at MY1 where it shows underestimation. Considering the average R-values (0.79–0.88), the predictions of the models show high correlations with the observations. Overall, the SVM models show a slightly different behaviour where it shows relatively poorer performance than the ANN and BRT models in the predictions of PM_{10} while it shows similar performance in the case of $PM_{2.5}$ predictions. The reason for this behaviour could be that the SVM overfitted the PM_{10} data as such it failed to generalise the performance gained during the training.

3.4. Emission estimates for EUROIV/VI scenario

Considering the period between 2011 and 2015, The projected traffic composition in central London (NAEI, 2014) shows that the percentage of petrol car was decreasing while the percentages of diesel car and electric vehicles were on the increase (see Table 5). However, there were no significant changes in the percentage of the other vehicles between this period. Also the percentage of diesel LGVs was much higher than that of the petrol LGVs and vice versa in the case of cars. The projected percentages of Taxi, Bus/Coach, HGVs and Motorcycles remained fairly the same between 2011 and 2015. The EUROIV/VI scenario restrictions were imposed on these traffic projections in 2011 and 2015 for PM_{10} models and 2012 and 2015 for $PM_{2.5}$ models.

Table 5
Projected traffic composition for central London (NAEI, 2014).

Year	Year_2011	Year_2012	Year_2015
Electric car	0.0%	0.0%	0.1%
Petrol car	40.1%	38.5%	34.0%
Diesel car	23.0%	24.6%	29.0%
Taxi (black cab)	12.4%	12.4%	12.4%
Electric LGV	0.0%	0.0%	0.1%
Petrol LGV	0.6%	0.4%	0.3%
Diesel LGV	11.2%	11.4%	11.4%
Rigid HGV	3.1%	3.1%	3.1%
Articulated HGV	0.4%	0.4%	0.4%
Bus and coach	4.2%	4.2%	4.2%
Motorcycle	5.1%	5.1%	5.1%

The variation in the base year was based on data availability.

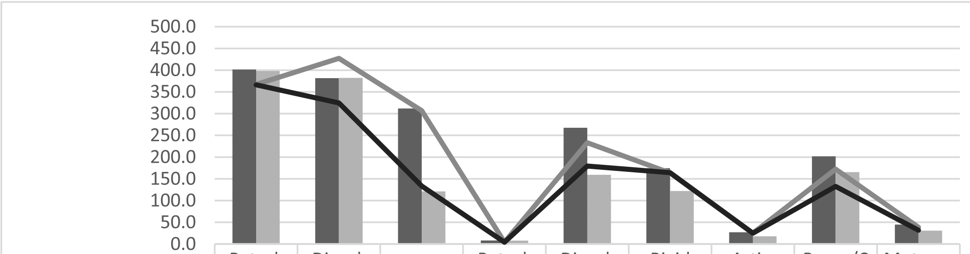
The PM_{10} emissions estimated with and without the scenario show that the emission from diesel cars, LGVs, Taxis, Bus/Coaches and HGVs has largely reduced due to the implementation of the EUROIV/VI scenario compared to the small reduction by the petrol vehicles (see Fig. 3). The total PM_{10} emission reduction due to the scenario in 2011 was 414.7 kg/yr out of which only 4.5 kg/yr was from the petrol vehicles. The PM emission in 2015 was generally lower compared to the year 2011. Also, In the year 2015, there was no reduction in the PM_{10} emission of petrol LGV, Rigid HGV and Articulated HGV. This behaviour could be attributed to the improvement in vehicle technology and the likely effect of the existing emission control strategies in London which might make the scenario to be less effective in 2015. However, the PM_{10} emissions from the London Taxi show the highest PM_{10} emissions reduction of 173.2 kg/yr due to the scenario while PM_{10} emissions of the diesel LGV and Buses/Coaches were reduced by 39.7 kg/yr and 53.7 kg/yr respectively. Having large reduction from these vehicles is an indication of the large impact of the scenario if it were to be implemented in 2015, because they fall into a category of vehicles with high particle emissions.

Moreover, the scenario in 2012 and 2015 for the $PM_{2.5}$ emissions reduction shows the same trend as in the case of PM_{10} with one important difference where there was $PM_{2.5}$ emissions increase of 1.7 kg/yr in 2012 and 62 kg/yr in 2015 by diesel cars (see Fig. 4). Overall, the implementation of the scenario resulted in higher reductions in the emissions of Taxis, diesel LGV and Buses/Coaches.

3.5. Performance of the ML models in predicting the effect of EUROIV/VI scenario

The models were first used to predict the particle concentrations in 2011 and 2015 without the EUROIV/VI scenario. The ANN and BRT models predicted that in 2015, without the EUROIV/VI scenario the annual mean concentrations of PM_{10} at the sites will be reduced by 0.86μg/m^3 – 5.35μg/m^3 across the sites (see Fig. 5). Also, they predicted that the number of days where PM_{10} was greater than 50μg/m^3 will be reduced by 3–26 days across the sites. The sites with higher traffic volume (MY1, BT4 and GR8) have shown higher reductions than the remaining sites. In both cases, SVM models predicted much higher reduction than ANN and BRT models which is not realistic considering the amount of decrease in the emission rates. The reduction shown by the ANN and BRT between 2011 and 2015 might be due to the current implementation of various emission control strategies put in place in London and the continuous improvement in the vehicle technology due to strict regulations on particle emissions.

When the scenario was implemented using data collected in 2011, the models predicted a slight reduction in the annual mean PM_{10} concentrations and the number days where PM_{10} was greater than 50μg/m3 as shown in Fig. 6. ANN and BRT models predicted that the annual mean PM_{10} concentrations will be reduced by 0.04–8.2 μg/m3 depending on the site. However, at KC2, the ANN model predicted that



	Petrol Cars	Diesel Cars	Taxi	Petrol LGV	Diesel LGV	Rigid HGV	Artic HGV	Buses/Coaches	Motorcycles
Year_2011	401.5	381.8	311.9	8.2	267.4	174.5	27.2	201.8	44.9
EUROVI_2011	398.2	382.1	121.1	8.0	159.3	122.0	17.9	165.5	30.8
Year_2015	367.0	427.2	306.8	4.3	233.2	163.5	24.9	172.4	38.6
EUROVI_2015	366.3	324.5	133.6	4.3	179.5	164.2	24.9	132.7	31.7

Fig. 3. Estimated annual PM_{10} emission rates (kg/yr) with and without EUROIV/VI scenario for MY1.

the annual mean PM_{10} concentrations would have been increased by 7.3 μg/m^3 while BRT model show that the concentrations would increase by 1.2 and 0.6 at CR4 and KC5 sites respectively. The SVM models predicted a much larger increase in the annual concentrations at all the sites despite the decrease in the emission rates.

The ANN and SVM predicted an increase in the PM_{10} concentrations in 2011 with the implementation of the scenario at KC2 while BRT predicted a slight reduction. This failure in the case of ANN and SVM might be attributed to the amount of missing values imputed in the data used for the training of the models. The data captured at this site in 2011, was 73%, and after the imputation, there were twenty eight days when PM_{10} concentrations were higher than 50μg/m^3 as against the seven days in the original data. Also, the 95 and 99 percentiles increased by 10μg/m^3 in the imputed data. Therefore, the performance of the models might be affected as the imputation heavily influenced the original data.

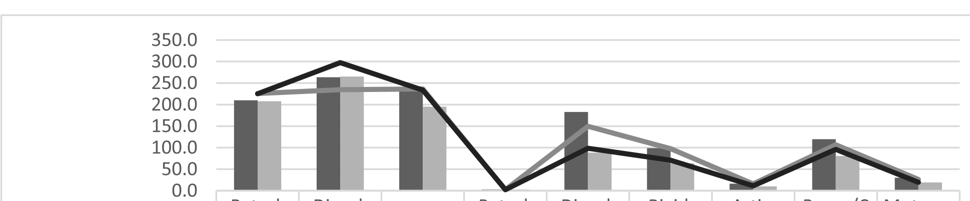
In the same year the ANN and BRT models predicted various degrees of reduction in the number of days where PM_{10} concentrations were higher than 50 μg/m^3 except at CR4 and KC5 where BRT predicted increase. Also, at KC2 the ANN model predicted an increase of 12 days. However, SVM models consistently predicted large increase at the sites.

When the scenario was implemented using 2015 data, the ANN and BRT predicted that the annual mean PM_{10} concentrations will be reduced by 0.14–2.18 μg/m^3 as shown in Fig. 7. They predicted high reduction at most of the sites except at GR5, KC5 and MY1 where they predicted less than 0.3 μg/m^3 reduction. At the BT4, GR5, and KC5 sites, the two models show approximately the same performance. Moreover, At CR4 site, the BRT model predicted a decrease of 6 μg/m3 which is unusually high compared with the results of the remaining models. However, in the case of number of days with PM_{10} greater than 50μg/m^3, BRT and ANN predicted different reductions at most of the sites except at BT4 and KC2. The SVM models predicted higher increase all the sites except at CR4 where it predicted reduction of 3 days.

The EUROIV/VI scenario explained above was also applied in predicting the concentrations of $PM_{2.5}$ in 2012 and 2015. The ML models predicted reduction of the annual mean $PM_{2.5}$ concentrations ranging between 0.3 μg/m^3 at GR9 to 2 μg/m^3 at MY1. In most cases, the predictions of the ANN and SVM were similar while BRT shows slightly different results. The same trend was also observed when the scenario was implemented in 2015 where they predicted higher reduction at MY1 and GR8 as shown in Fig. 8 (middle).

All the models predicted a reduction in the concentrations from 2012 to 2015 (see Fig. 8 right), even though there was an increase in traffic volume. The reduction might be attributed to the improvement in the vehicle technology and other air quality control measures being implemented in London (TFL, 2016).

The ML models are data driven, and they are trained to mimic the observed data based on the relationships they derive from predictor variables and the response variables data. Therefore, their performance will largely depend on the accuracy and completeness of the data. The models have shown good performance in predicting the particle concentrations. Their poor performance, where it occurred, could be mostly attributed to their inability to capture the extreme events such as extremely high or low concentrations that are rarely happening in most of the sites. This behaviour is not unexpected as they have some element of statistics in their formulation that has a bias towards the most frequent events. Another reason that will also contribute to their poor performance is the amount of missing data in the training and testing data. An attempt has been made to reduce this effect by using some missing data imputation algorithms. The SVM models show different prediction behaviour compared to the BRT and ANN models where they predicted increase in the PM_{10} statistics at most of the sites.



	Petrol Cars	Diesel Cars	Taxi	Petrol LGV	Diesel LGV	Rigid HGV	Artic HGV	Buses/Coaches	Motorcycles
Year_2012	210.1	263.6	233.7	3.0	182.9	98.9	16.4	119.7	30.3
EUROVI_2012	208.0	265.3	195.4	2.9	88.5	63.7	10.1	80.5	19.2
Year_2015	225.7	234.7	236.4	2.3	149.5	97.7	15.9	106.9	26.2
EUROVI_2015	225.0	297.5	233.5	2.3	98.7	70.8	11.3	96.1	19.7

Fig. 4. Estimated annual $PM_{2.5}$ emission rates (kg/yr) with and without EUROIV/VI scenario for MY1.

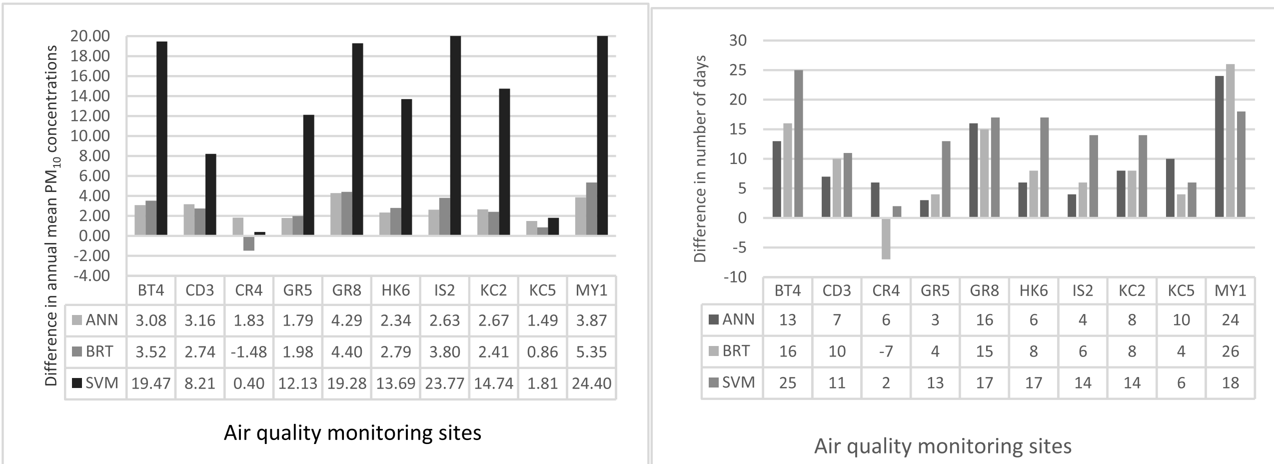


Fig. 5. The difference between the prediction of the models from 2011 to 2015 without the scenario. The annual mean PM_{10} concentrations (left) and a number of days where PM_{10} is greater than 50μg/m3 (right).

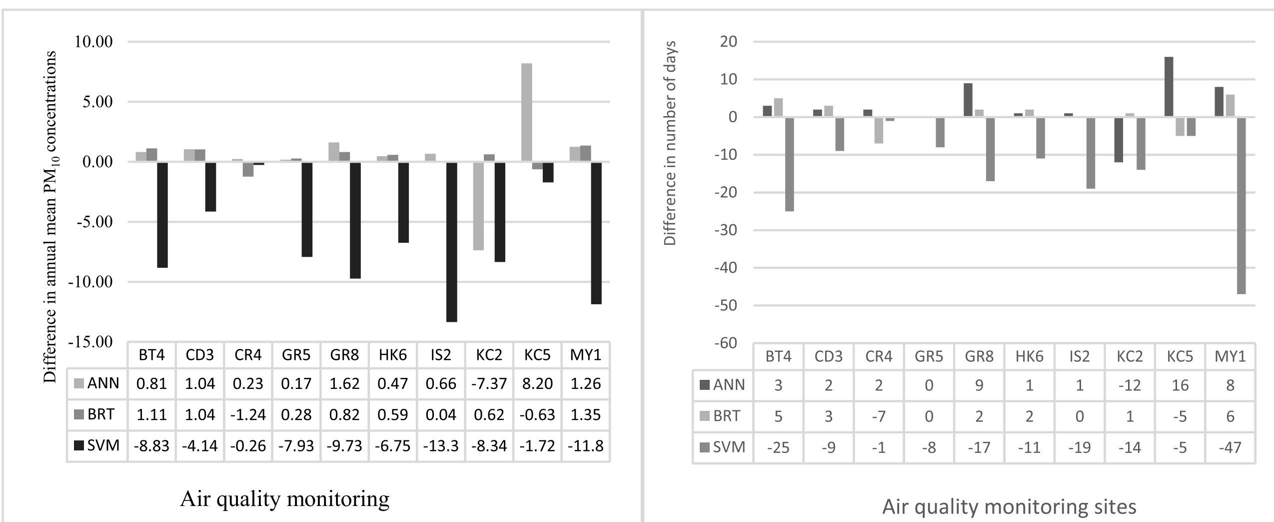


Fig. 6. The difference between the prediction of the models with and without the scenario in 2011. The annual mean PM_{10} concentrations (left) and the number of days where PM_{10} is greater than 50μg/m^3 (right).

However, they performed similarly in the case of $PM_{2.5}$. The reason for this behaviour could not be reliably established, but it was suspected that the models might have overfitted the training data and subsequently failed to generalise the performance.

4. Conclusions

This paper explores the use of machine learning models in air quality management. The performance of the models in predicting PM_{10} and $PM_{2.5}$ concentrations at twelve monitoring sites in London was compared. Also, the performance of the models in evaluating the effect of a hypothetical air quality management scenario on roadside particle concentrations, PM_{10} and $PM_{2.5}$ was compared. The ANN and BRT performed better than the SVM in predicting PM_{10} concentrations while they vary only little in their performance when predicting $PM_{2.5}$ concentrations.

The ANN method selected traffic emissions from various vehicles as the most contributing variables followed by the roadside and background oxides of nitrogen, temperature, wind directions and temporal variables respectively. The BRT method gave preference to the roadside and background concentrations of oxides of nitrogen and background particle concentrations while indicating similar but lower contributions from the remaining variables. Combining the information gained from the two methods, the traffic, roadside and background concentrations of gaseous pollutants could help in determining the levels of roadside particle concentration. Therefore, it is recommended that relevant environmental agencies and other stakeholders should maintain more quality data on these variables so that they can be used in training ML models to effectively manage the roadside concentrations of PM_{10} and $PM_{2.5}$. Also, oxides of nitrogen were seen to be highly correlated with the PM_{10} and $PM_{2.5}$. Therefore, effective monitoring and control of these pollutants might help in managing the particle concentrations.

When evaluating the effectiveness of the EUROIV/VI scenario, the ANN and BRT models predicted reductions in the PM_{10} and $PM_{2.5}$ concentrations. While in a few cases, they predicted that the concentrations will remain unchanged. The SVM model consistently predicted higher PM_{10} concentrations when tested with the scenario while predicting a much smaller decrease in $PM_{2.5}$ concentrations. However, it predicted a much larger decrease in PM_{10} concentrations in 2015 without the scenario. According to all the performance metrics used in this study, the SVM model was the poorest in predicting PM_{10} whereas it shows similar performance with ANN and BRT in predicting $PM_{2.5}$. This behaviour could be attributed to overfitting during SVM training, however, this study recommends that the application of SVM method in

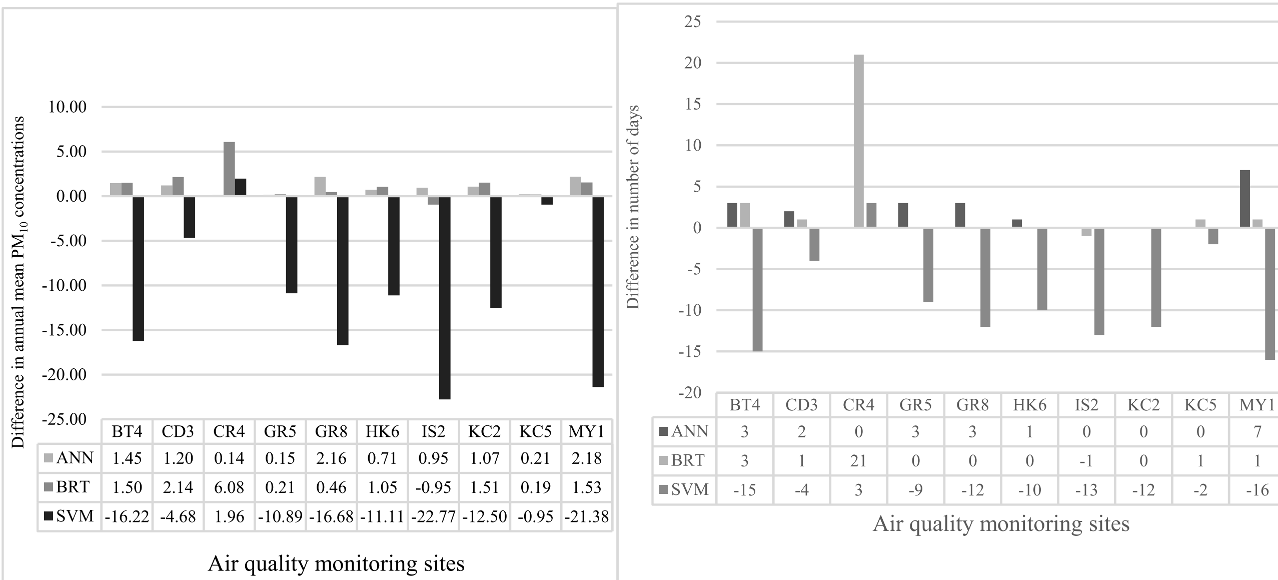


Fig. 7. The difference between the prediction of the models with and without the scenario in 2015. Annual mean PM_{10} concentrations (left) and the number of days with PM_{10} greater than 50μg/m^3 (right) in 2015.

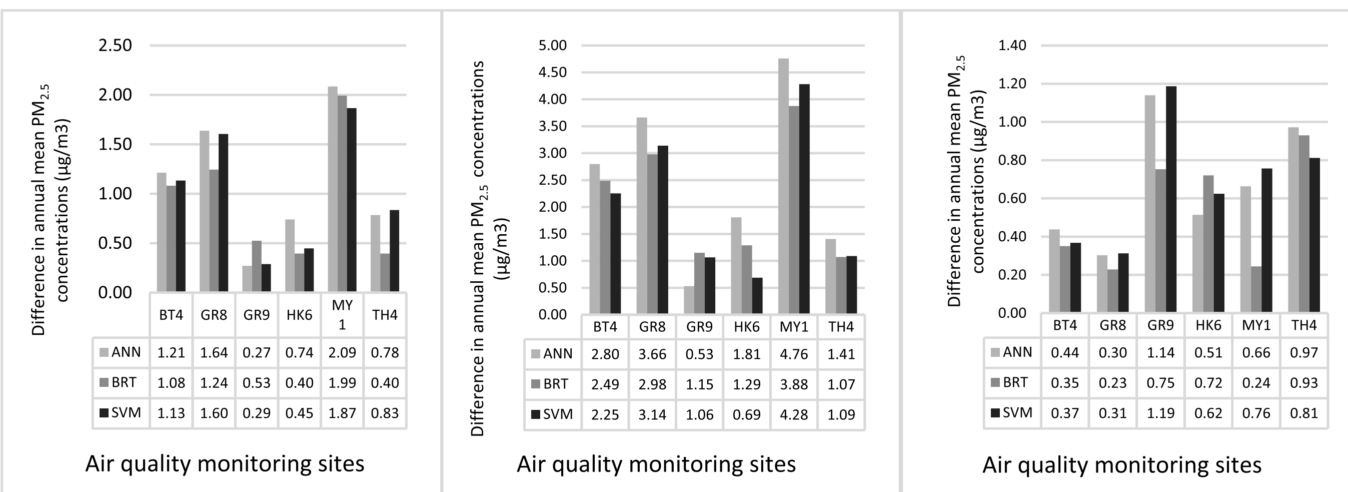


Fig. 8. Predicted change in the annual mean $PM_{2.5}$ concentrations in 2012 (left), 2015 (middle) and the predicted change in the annual mean $PM_{2.5}$ concentrations from 2012 to 2015 (right).

air quality management should be further investigated.

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