Dispersion Modeling of Air Pollutants in a Hilly City in India

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Abstract: Vehicular pollution is one of the major sources of air pollution in urban locales that have reportedly elevated concentrations of air pollutants. This study aims to examine the performance of two air quality dispersion models, STREET and CALINE 4 to predict pollutant concentrations for an urban monitoring location that is en route to the high traffic volumes in Shimla, Himachal Pradesh, India. This study will compare the predicted and observed concentrations (for the urban monitoring location) using both quantitative and statistical methods for the 2 years of the study. The pollutant selected for the study is PM_{10}. It was observed from the modeling studies that the performance of CALINE4 was slightly better than the STREET model. The models selected to a certain extent are defined by the available parameters for successful run completions. The application of detailed modeling studies is the first of its kind for the study location, to the best of the authors' knowledge. Hence, the application of basic and simplistic models and the examination of their performance could potentially find the best fit model to predict approximately precise concentrations. Further scope of this study should include the use of advanced air quality dispersion models for the improved prediction of concentrations. **DOI: 10.1061/(ASCE)HZ.2153-5515.0000574**.

Author keywords: Air quality dispersion models; CALINE 4; STREET; Shimla.

Introduction

India is one of the fastest growing economies in the world. The rapid growth through industrialization and globalization has been followed by increasing population and urbanization. These factors are of prime concern for every country that places a burden on the natural resources and deposits on the earth (EEA 2013). In particular, air quality degradation in urban areas is the result of increased anthropogenic activities, primarily automobiles and industrial activities. Recently, there has been a significant drop in pollution due to industrial and domestic activities as a result of interventions by concerned regulatory bodies in central and state governments (Sharma and Khare 2001; Nagendra and Khare 2002). However, a significant increase in population has created the demand to meet the need for transportation. The increase in the number of motor vehicles has led to a substantial increase in air pollution caused by vehicular exhaust emissions (VEE) (Nagendra and Khare 2002). It has been universally acknowledged that directly generated VEEs or those indirectly produced through photochemical reactions pose a significant threat to human health (Vardoulakis et al. 2003; Ganguly and Broderick 2008; Guttikunda and Goel 2013). Therefore, even if the introduction of vehicles with strict emissions could reduce the overall pollutant emissions, the increase in the number of vehicles could neutralize this impact in overall emissions (Sharma and Pundir 2008; Hama et al. 2020).

Therefore, the potential effects of the pollutants on human health and environment have created an immediate need for the assessment of ambient air quality. Developing a mathematical model is one type of approach that could be used to analyze the impacts of air pollution, retrospectively and prospectively. Moreover, government departments and agencies have started relying on these models for policy-making decisions for air quality and traffic management, urban planning, and public health. Air quality models provide theoretically estimated information for the air pollution levels as well as spatial and temporal variations (Sharma and Khare 2001).

Air quality dispersion modeling is an important tool when depicting the contribution and impacts of road traffic emissions on air quality. The pollutant concentration predictions in the model are functions of meteorological conditions, highway geometry, and receptor location. The road traffic concentrations are combined with the background concentrations of pollutant to obtain total concentrations, which decrease as a function of the distance from the road (Ganguly and Broderick 2010a; Ganguly et al. 2015). The diversity and quantity of vehicle numbers directly account for the rate of VEEs on the street. Therefore, evaluation of the emission factor is a crucial component of the air quality dispersion model, because it accounts for vehicles and the dispersion of pollutants that could affect the veracity of predictions.

In a previous study, we presented the preliminary and basic details for a long-term analysis of particulate matter concentrations for the city of Shimla and discussed the insufficient number of monitoring stations in the city (Ganguly et al. 2019). The previous study reported the inadequate number of monitoring stations that exist in Shimla to accurately represent the air quality data. In particular, the presence of adequate monitoring stations, and therefore, the monitored data were used to classify the air quality monitoring objectives (both short- and long-term implications), the existing ambient air quality, and evaluating the effectiveness of different air quality abatement programs. However, it is noted that the monitored air quality data often suffer from certain drawbacks that include the scarcity of full time operational monitoring stations and unreliable representation of spatial patterns (Batterman et al. 2015).

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Air quality dispersion models based on the Gaussian Plume Model (Snyder et al. 2013), land use regression (LUR) (Hoek et al. 2008), hybrid (Gokhale and Khare 2005; Ganguly and Broderick 2010b), and receptor (Taiwo et al. 2014) modeling approach are often employed to assess the temporal and spatial patterns of air pollutants from vehicular sources.

Dispersion of air pollutants in complex hilly terrains is different from and much more complicated than in flat areas due to orographic atmospheric interactions at various spatial scales (Giovannini et al. 2020), nonhomogenous atmospheric fields that are characterized by synoptic forces, mesoscale circulations and turbulence fluctuations (Giovannini et al. 2020), and inaccuracies in model structures (Dhyani et al. 2013; Podnar et al. 2002). Further, the use of Gaussian-based dispersion models on the street canyon hypothesis is often not deemed suitable for use in hilly areas since only a windward or leeward side exist, not both. In addition, due to the existence of almost calm conditions, the application of Gaussian equation-based models are often not preferred (Kim and Lee 1998). These models yield approximate results without a detailed study of roadside particulate matter plume movement and dust resuspension (Srimuruganadam and Nagendra 2010).

Considering the previous points, a significant amount of scientific research has been carried out using dispersion models for complex terrains. For example, Venkatram et al. (2001) demonstrated the process of model development to estimate the pollutants levels associated with complex terrains areas. Ritter et al. (2013) investigated the application of WRF-Chem over very complex terrain in Switzerland and compared the results with PolluMap, a Gaussian model. It was observed that the Gaussian model performed slightly better than the WRF-Chem model for NO_2 and PM_{10}. Tomasi et al. (2019) compared two different sets of dispersion models CALMET/CALPUFF (Gaussian model) and WSI/SPRAY-WEB (Lagrangian model), under the Bolzano Tracer Experiment over the Eastern Italian Alps. The statistical analysis highlighted the better performance of the Lagrangian model compared with the Gaussian model.

In the previous studies, the Gaussian-based dispersion model in hilly or complex terrains was applied. However, the dispersion models, such as AERMOD and CALMET/CALPUFF are advanced versions of Gaussian-based models, but the fundamental underlying principles are similar to the those applied in CALINE 4. CALINE 4 uses the simplest of the input parameters, and the previously discussed Gaussian-based models, such as AERMOD, and CALMET/CALPUFF use more detailed data for emission inventory, meteorology, and terrain inputs.

In addition, the application of Gaussian-based dispersion models have previously been used in complex Indian terrains for the analysis of ambient air quality; however, the reliability of the results remains in the application of these models. For example, Dhyani et al. (2013) showed the unsatisfactory performance of CALINE in hilly terrain conditions; however, the study stated the need for emission factors that satisfy the variable vehicle speed and gradient conditions. Similarly, a study conducted by Goyal et al. (2006) highlighted the satisfactory performance of Gaussian models to compute the concentrations of criteria pollutants SO_2, SPM, and NO_x in the hilly city of Gangtok. This shows the successful application of a Gaussian dispersion model in hilly and complex terrain. The quality of the model results depend on the input parameter and more advanced dispersion models require more accurate input data; however, the application of Gaussian-based simple dispersion models in hilly areas should not be discounted, because in developing countries the availability of limited input data is a significant constraint for complex advanced models.

This study describes an assessment of PM_{10} predictions at an urban street canyon site in Shimla, Himachal Pradesh, (India) using two Gaussian-based dispersion models STREET and CALINE 4. The models were selected for the study location based on their simplicity and ease of operability. No modeling analysis has previously been performed for the study location, to the best of the authors' knowledge. Therefore, modeling work will be undertaken by the authors as an initial assessment to predict the pollutant concentrations at the study location. Air quality data obtained for 2015–2016 is compared with the predicted data obtained using the two models. The statistical evaluation of the models and their prediction performances on daily average PM_{10} concentrations is illustrated.

Methodology

Study Locations

The primary location for this study was Shimla, which is the capital of the state of Himachal Pradesh situated 2,000 m above mean sea level (MSL) in the middle Himalayas range. The city lies in a cold and cloudy climate zone that has fairly long winters from October to March with severe cold spells for 2 months (January and February) when temperatures almost reach 0°C. The summer months (May–June) are pleasant with maximum temperatures of approximately 30°C. The monsoon period (July and August) result in heavy rainfall that might lead to humid conditions. The intervening months have a very mild climate. The following sections discuss some of the important contextual information regarding the study location.

Location of Street Canyon Section (Old Bus Stand)

The modeling study was carried out near the Old Bus Stand Junction within the city, which is a two-way two-lane road located in the very heart of Shimla and covers the main arterial road of the city. Figure S1 shows the general layout of the Old Bus Stand road. The average width (W) of the road was 8 m (Shekhar 2011) and the canyon height (H) was 12 m. Hence, the road cross section was classified as an intermediate street canyon with an aspect ratio (H/W) of 1.5, lying between the values of a regular canyon (H/W = 1) and a deep canyon (H/W = 2) (Vardoulakis et al. 2003). The other relevant pertinent details for the study location are discussed in the following sections.

Traffic Volume

The annual average daily traffic (AADT) data is an important factor when determining the emission factors as an input to the air quality dispersion models. However, there are no relevant studies or adequate records of data for the AADT values for the study period available from the local traffic authorities. The AADT values for different years were calculated by assuming a 10% increase every year after consulting the available literature. In a previous study the authors assumed a 10% increase every 5 years by applying the Transport Annual Guidance (WEBTAG) specification (Ganguly and Thapa 2016). Further, in a recent study, it was mentioned that the growth rate of vehicles in India is approximately 10% (Vijayalakshmi and Raj 2019), which supports the assumptions made by the authors. Finally, this traffic growth rate was discussed with the engineer for the Regional Transport Office (RTO) Shimla before finalizing the assumption (personal communication from the engineer of RTO, Shimla, 2015–2016). Using this assumption, the emission factor for the pollutant was determined as discussed in the following section.

Emission Factors

The appropriate determination of emission factors is one of the essential requirements when determining the pollution load produced and the amount of raw material burned that affect the accuracy of the predictions of the air quality model. For the road transport sector, it is defined as the ratio of the amount of pollution produced by the number of vehicle km traveled (Ganguly and Broderick 2010a). Emission factors employed in India do not depend upon speed and are based on the Indian driving cycle on a chassis dynamometer, which typically portrays the Indian driving conditions (CMVR 1989). The vehicular emissions are available for different categories of vehicles that mainly depend on the type and efficiency of fuel as well as type of engine, emission reduction measures, maintenance, and age of the vehicle (Ramchandra and Shwetmala 2009; Dhyani et al. 2013). The driving patterns for different cities can differ significantly; however, a city-specific emission factor has not been formulated in India (ARAI 2008). The development of city-specific emission factors would help to simulate improved real condition scenarios (ARAI 2008). In particular, we calculated the weighted emission factor (WEF) using the emission factors specified by the ARAI manual (ARAI 2008)

$$\mathrm{WEF} = \frac{\left[\sum N(j)\cdot EF(i,y)\right]}{\text{Total number of vehicles}} \tag{1}$$

where WEF = weighted emission factor; $N(j)$ = a number of vehicles of a particular type j; and $EF(i,j)$ = emission factor of a pollutant i for the jth vehicle type. Using Eq. 1 the emission factors were determined to be 0.48 g/km (0.78 g/mile) and 0.54 g/km (0.87 g/mile) respectively for 2015 and 2016, respectively.

Measurement of PM_{10} Concentration

The concentrations of pollutant PM_{10} were measured using a respirable dust sampler with a cyclonic connector with an airflow rate of 1.1 m^3/min. The amassed particulate matter was collected on a filter paper and then the mass retained was determined in the laboratory, which was divided by sample air volume and reported in parts per million units. The monitoring programs carried out at the location in the study area adhered to the Central Pollution Control Board (CPCB) regulations and were maintained by the Himachal Pradesh Pollution Control Board (HPPCB). There are two stations where the HPPCB carries out monitoring studies: one is Tekka Bench, at the Ridge that was designated as the background site (Monitoring Station I) and the Old Bus Stand monitoring station that was identified as the commercial combined with residential site, or the urban site (Monitoring Station II). The monitoring station at the Old Bus Stand is 7.92 m from the road level as shown in Figure S1. Figure S2 shows the monitoring equipment that has been installed at the bus stand site.

The data for the monitored PM_{10} concentrations were obtained from the HPPCB for 2011–2017. The long-term trend analysis for the city is explained in Ganguly et al. (2019). However, for this study, PM_{10} concentrations monitored for 2015 and 2016 were used to initiate the modeling work for the city. The daily average concentrations for 2015 varied between 23.59 and 118.65 $\mu g/m^3$ with an annual average of 69.27 ± 16.78 $\mu g/m^3$. However, for 2016 the daily PM_{10} concentrations fluctuated between 28.01 and 110.35 $\mu g/m^3$ with an annual mean concentration of 63.75 ± 17.22 $\mu g/m^3$. It was observed that concentrations of PM_{10} were highest during the summer season and lowest during the monsoon season for both years.

Meteorological Data

Meteorological parameters required for modeling were collected from the Indian Meteorological Department, Shimla, which has its monitoring station installed approximately 2.5 km from this study location. The meteorological parameters included wind speed and its direction, minimum and maximum temperature, precipitation, and relative humidity and visibility, which were then used as input for the selected models. Figures S3 and S4 show the windrose diagrams plotted for 2015 and 2016, respectively. The prevalent NE wind direction was observed throughout the study period. Calm conditions were prominent during approximately 83.7% for the study period (2015 and 2016). The average relative humidity and temperature for the study period were approximately 60% and 15.5°C, respectively.

Air Quality Dispersion Models

Two simple air quality dispersion models CALINE4 and STREET were selected for evaluation and application and the selected stretch of road on the study location. The primary reasons for the selection of the models were that very minimum input parameters are required for the models, which are highly effective in predicting concentrations. The two models (STREET and CALINE 4) used in this study are Gaussian Plume models that assume for a point source, concentrations are a function of emission rate, meteorological conditions (specifically wind speed), and receptor location (Awasthi et al. 2006). Additional details about these models are discussed in the following section.

CALINE 4

CALINE 4 is the latest version of CALINE series of pollutant dispersion models that have been developed by California Department of Transportation (Caltrans) (Benson 1984). It uses a Gaussian Plume dispersion equation to predict the line source emissions on the street. This model employs the concept of a *mixing zone* to characterize the dispersion of pollutants over the street. Mixing zone refers to the area that lies directly over the street, which is assumed to have turbulence and uniform emission rates. It is a computer-based model that can be employed to predict the concentrations of several pollutants especially CO, NO_x, inert gases, and particulates (Benson 1992; Sharma and Khare 2001; Ganguly et al. 2009). It can be used for various road circumstances and conditions that include intersections, bridge, and depressions.

The major requirements of the CALINE 4 model is the road geometry, such as roadway height, receptor locations and heights, number of links, and mixing zone width as input (Benson 1984; Goud et al. 2015). The roadway is divided into a series of elements and then individual concentrations of these segments are calculated using the Gaussian dispersion equation and then combined to form a total concentration. The Gaussian equation used for any pollutant at any point (x, y, z) can be written as follows:

$$C = \frac{q}{2\pi u\sigma_y\sigma_z}\left\{\begin{array}{l}\exp\left[\dfrac{-(z-H)^2}{2\sigma_z^2}\right]\\ +\exp\left[\dfrac{-(z+H)^2}{2\sigma_z^2}\right]\end{array}\right\}\int_{y1}^{y2}\exp\left(\frac{-y^2}{2\sigma_y^2}\right) \tag{2}$$

where q = line source strength; U = wind speed; σ_z and σ_y = vertical and horizontal Gaussian dispersion parameters that are functions of x, not y; H = height of source; σ_y and σ_z are calculated using the Pasquill's stability class. The application of CALINE 4 for street canyons has been limited (Vardoulakis et al. 2003).

STREET

The term *street canyon* is defined as a narrow street that has buildings continuously along both the sides (Nicholson 1975). However, in reality, the term applies to urban streets that do not necessarily have buildings continuously on both sides (Vardoulakis et al. 2002, 2003).

It is one of the earliest and simplistic models that uses initial dispersion and car induced turbulence to calculate a series of hourly concentrations at different receptor locations within a canyon (Johnson et al. 1973). The pollutant concentration generated within a canyon was presumed to consist of two components, the urban background concentrations component (C_b) and the concentration component (C_s), caused by vehicular emissions generated within the street

$$C = C_s + C_b \tag{3}$$

The C_s component is derived from a simple box model (Johnson et al. 1973). It is composed of two elements the leeward (the side of the street from which roof wind blows) and windward side (the side of the street to which the wind blows at roof level) concentrations. The former depicts the build-up and intensification of pollutant and the latter represents the pollutant concentration developed from recirculation in the street (Ganguly and Broderick 2010a). The leeward side concentrations are given by the following expression:

$$C_S^L = \frac{KQ}{(U + U_s)\left(\sqrt{x^2 + z^2} + h_o\right)} \tag{4}$$

where K = empirical constant parameter; Q = rate of emission discharge in street; U = roof level wind speed; U_s = constant that accounts for additional movement of air induced by movement of traffic (empirical value 0.5 m/s); x = horizontal distance of receptor from center of traffic lane; z = receptor height; h_o = constant that represents initial pollutant dispersion height (empirical value 2 m). The K value can be determined for particular site-specific conditions, but general values of the constants have been found to vary between six and eight. The studies conducted previously using the STREET model demonstrated that the use of the K value was satisfactory. Qin and Kot (1993) calculated the value of K to be six for their work in a street canyon in China. A study conducted in Dublin, Republic of Ireland by Ganguly and Broderick (2010a) determined the value of K to be seven. A K value of eight was observed in Buenos Aires, Argentina by Bogo et al. (2001). In our study, modeling assessments were carried out using different values of K between 6 and 8, with the most optimal results observed for values of $K = 7$.

The original expression given to calculate concentrations on the windward side by Johnson et al. (1973) was revised by Dabberdt et al. (1973) to take into consideration the vertical decrease in pollutant concentrations that occurred due to fresh air entrainment from the top of the canyon. The final equation derived to calculate the concentrations of the windward side was

$$C_S^W = \frac{KQ}{W(U + U_s)}\left(\frac{H - z}{H}\right) \tag{5}$$

where H and W = the height and width of the canyon. STREET is an empirical model; however, the significant features of pollutant dispersion in street canyons are described by Eqs. (2) and (3) (Berkowicz 1997). The average of Eqs. (4) and (5) should be calculated for parallel or near parallel wind conditions. With some minor modifications, the model is still widely used, especially for engineering applications (Kumar et al. 2009).

Modeling Conditions Used in This Study

As explained in the section "Study Locations," one of the main assumptions made for this study was a 10% increase in a number of vehicles per annum. To determine the best modeling predictions for the study location, four conditions were used, which appear to be reasonable conditions to conduct the modeling studies. These conditions were:

1. Prediction of concentrations at Monitoring Station II using mean background concentrations at Monitoring Station I [designated background site (Case I)].
2. Prediction of concentrations using nighttime (10:00 p.m.–6:00 a.m. local time) background concentrations of Tekka Bench monitoring station (Case II).
3. Prediction of concentrations using nighttime (10:00 p.m.–6:00 a.m.) concentrations at the urban site as background concentration (Case III).
4. Prediction of concentrations by using vehicle proportioned nighttime (10:00 p.m.–6:00 a.m.) concentrations at the urban site as background concentrations. To conduct modeling studies under this condition, traffic volume studies were conducted for 7 days consecutively at Monitoring Site II and the time when the lowest vehicle count occurred was determined. Then, using the proportion method, the lowest concentrations that could occur during that time was found and used for modeling (Case IV).

Due to the unavailability of data related to some parameters, such as settling and deposition velocity and mixing zone height, default values were used for model prediction, an assumption that has previously been used and reported in earlier literature (Gokhale and Raokhande 2008; Holnicki and Nahorski 2015).

Statistical Parameters for Model Evaluation

The operational efficiency of any model can be evaluated by the comparative analysis of predicted concentrations for the monitored concentrations using relevant statistical measures. Willmott (1981) and Marmur and Mamane (2003) have given a comprehensive interpretation regarding the use of the appropriate statistical parameters for the comparative analysis. Table 1 describes the statistical parameters used with the methods for calculating them that are primarily based on the parameters described by Chang and Hanna (2004).

The index of agreement (IA) determines the parity, which is simply the degree of similarity between monitored and modeled concentrations Willmott (1981). An IA value of one corresponds to the perfect agreement between the monitored and predicted concentrations. The normalized mean square error (NMSE) highlights the scattering in the data set (Kumar et al. 2008). It gives the particulars regarding the error that could be produced by the model. Pearson's correlation coefficient (R) is a measure of linear dependency between two variables. However, it cannot differentiate the size and type of covariance of the datasets. Fractional bias is a numerical quantity, which is used as a measure of agreement between mean concentrations to disclose the amount of overestimation or underestimation (EPA 2000). A factor of two statistically is indicative of the level of prediction of the model.

Results and Discussions

The results and discussions for the modeling applications were discussed in four different cases that were described in the section "Modeling Conditions Used in the Study" previously. Further, it was observed that values of short-term, as well as long-term average parameters, were almost identical for all three K values that varied between 6 and 8. Hence, the STREET modeling results are represented based on $K = 7$ conditions.

Table 1. Statistical parameters used for performance evaluation

Statistical parameter	Formula	Min	Max	Ideal
Mean	$\bar{C} = \sum_{i}^{n} C_i / n$	—	—	—
SD	$\sigma = \sqrt{\frac{1}{n} \sum_{i-1}^{i=n} (C_i - \bar{C})^2}$	—	—	—
IA	$\text{I.A.} = 1 - \frac{\overline{(C_{\text{pred}} - c_{\text{obs}})^2}}{\overline{(\lvert C_{\text{pred}} - \overline{C_{\text{obs}}}\rvert + \lvert C_{\text{obs}} - \overline{C_{\text{obs}}}\rvert)^2}}$	0	1	1
NMSE	$\text{NMSE} = \frac{\overline{(C_{\text{pred}} - C_{\text{obs}})^2}}{\overline{C_{\text{obs}}}\,\overline{C_{\text{pred}}}}$	0	∞	0
Pearson's coefficient of regression (R)	$R = \frac{\overline{(C_{\text{obs}} - \overline{C_{\text{obs}}})\,(C_{\text{pred}} - \overline{C_{\text{pred}}})}}{\sigma_{\text{pred}}\sigma_{\text{obs}}}$	−1	1	0
Fractional bias (FB)	$\text{FB} = \frac{2(\overline{C_{\text{pred}}} - \overline{C_{\text{obs}}})}{\overline{C_{\text{pred}}} + \overline{C_{\text{obs}}}}$	−2	2	0
Factor of two (FAC_2)	$\text{FAC}_2 = 0.5 < \frac{C_{\text{pred}}}{C_{\text{obs}}} < 2$	0	1	1

Note: FAC_2 = factor of two; FB = fractional bias; IA = Index of Agreement; NMSE = Normalized Mean Square Error; R = Pearson's coefficient of regression; SD = standard deviation; n = total number of observations; C_i = concentration of ith observation; $\bar{C}$ = mean concentrations of n observations; σ = standard deviation; C_{pred} = predicted concentrations; C_{obs} = observed concentrations; σ_{pred} = predicted standard deviation; and σ_{obs} = observed standard deviation.

Table 2. Comparative analysis of model predictions for PM_{10} using average background conditions from Monitoring Station II for 2015 (Case I)

Statistical parameters	Monitored concentrations	Modeled concentrations (CALINE 4)	Modeled concentrations (STREET) $K = 7$
Mean	70	45	41
Systematic bias	—	25	29
SD	16	15	14
R	1.00	0.24	0.29
FB	0.00	−0.44	−0.51
NMSE	0.00	0.31	0.39
IA	1.00	0.44	0.57
FAC_2	1.00	0.79	0.70

Note: FAC_2 = factor of two; FB = fractional bias; IA = Index of Agreement; NMSE = Normalized Mean Square Error; R = Pearson's coefficient of Regression; SD = standard deviation.

Table 3. Comparative analysis of model predictions for PM_{10} using average background conditions from Monitoring Station II for 2016 (Case I)

Statistical parameters	Monitored concentrations	Modeled concentrations (CALINE 4)	Modeled concentrations (STREET) $K = 7$
Mean	64	47	43
Systematic bias	—	17	21
SD	18	13	13
R	1.00	0.47	0.50
FB	0.00	−0.31	−0.39
NMSE	0.00	0.19	0.25
IA	1.00	0.58	0.44
FAC_2	1.00	0.91	0.86

Note: FAC_2 = factor of two; FB = fractional bias; IA = Index of Agreement; NMSE = Normalized Mean Square Error; R = Pearson's coefficient of Regression; SD = standard deviation.

Modeling Assessment for Case I Conditions

The modeling results for this case are presented in Tables 2 and 3, respectively for 2015 and 2016 at Monitoring Station I. The scatter plots of modeled and predicted data are shown in Figs. 1 and 2 for 2015 and 2016, respectively. The main assumption utilized when carrying out the modeling analysis was that the background concentrations were considered to be the average of the entire monitoring concentrations obtained from Monitoring Station II during the study period. It was observed that IA values were comparatively higher for STREET (IA = 0.57) than CALINE 4 (IA = 0.44) for 2015 and the reverse was observed for 2016. Similarly, the correlation parameters were slightly higher for STREET compared with CALINE 4 for both years. However, the NMSE values were slightly better for CALINE 4 compared with STREET model for both years. Further, the predicted concentrations using the average background concentrations were 1.5–1.7 times less than the monitored concentrations that demonstrated severe under predictions. The short-term model performance parameters vary from model to model and year to year; however, for long-term model assessment, the CALINE 4 model was slightly better than the STREET model. Further, the modeling results obtained using these assumptions indicated that the average background levels from Monitoring Station II (which is a designated background site) were not a suitable representation of the actual background concentrations for the pollutants.

Modeling Assessment for Case II Conditions

Similar to Case I, the modeling results for this case are summarized in Tables 4 and 5, respectively for 2015 and 2016 at Monitoring Station I and the scatter plots for the monitored and predicted results are shown in Figs. 3 and 4. The main difference in the assumption utilized when carrying out the modeling analysis for Case II was that for Case I the entire average of the concentrations from Monitoring Site II was treated as the background concentration whereas in Case II the average concentrations that covered only the nighttime concentrations from Monitoring Site II were considered for the background concentrations. The main reasoning behind this assumption was that during this period

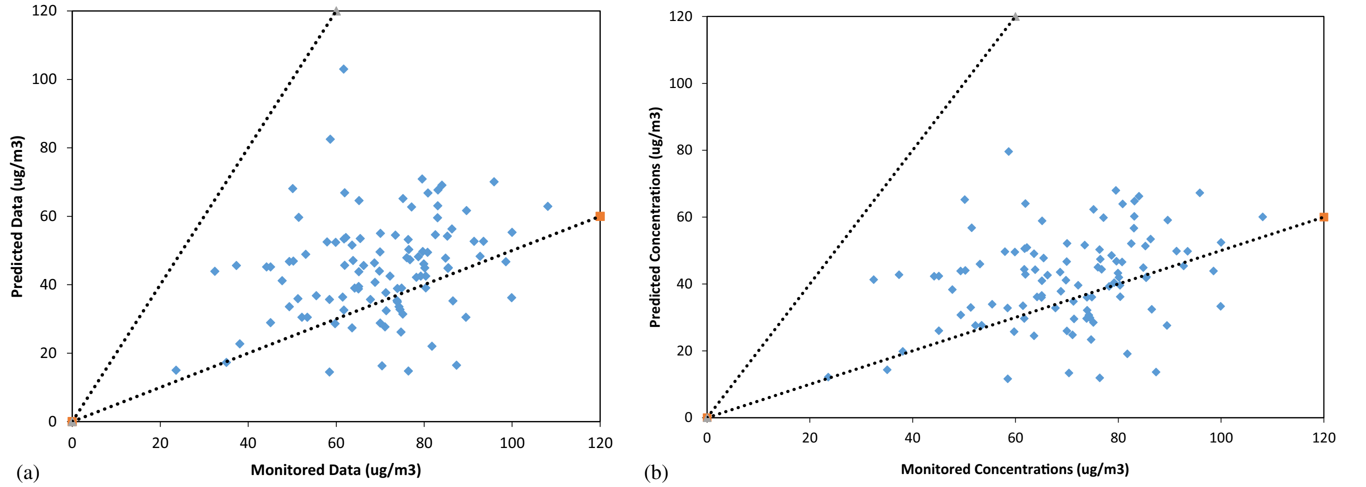

Fig. 1. Scatter plots of modeled and predicted data for PM_{10} using average background conditions from Monitoring Station II for 2015 (Case I) using; (a) CALINE 4; and (b) STREET.

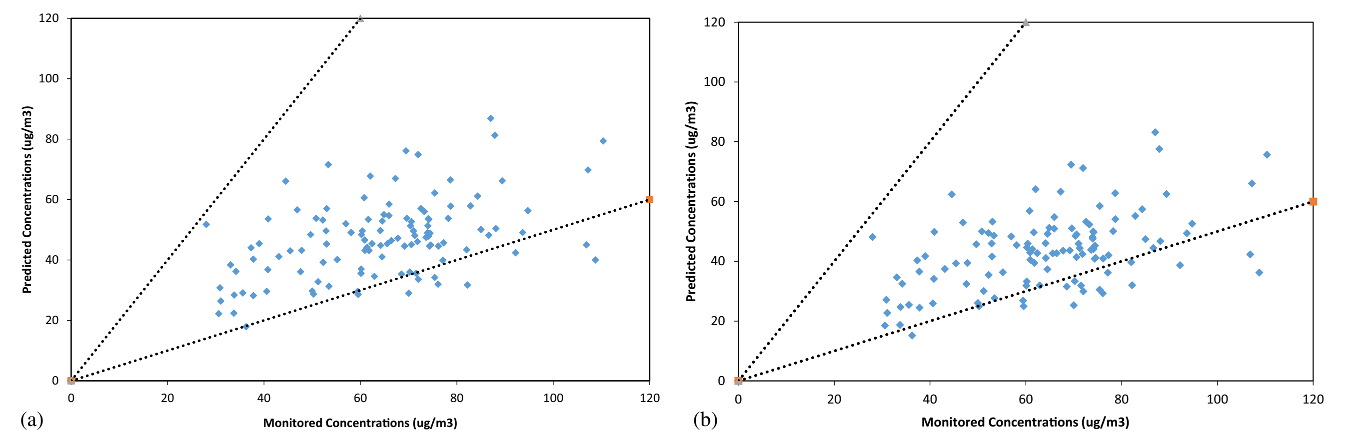

Fig. 2. Scatter plots of modeled and predicted data for PM_{10} using average background conditions from Monitoring Station II for 2016 (Case I) using: (a) CALINE 4; and (b) STREET.

Table 4. Comparative analysis of model predictions for PM_{10} using nighttime background conditions (10:00 p.m.–6:00 a.m.) from Monitoring Station II for 2015 (Case II)

Statistical parameters	Monitored concentrations	Modeled concentrations (CALINE 4)	Modeled concentrations (STREET) $K=7$
Mean	70	43	38
Systematic bias	—	27	32
SD	16	19	18
R	1.00	0.23	0.27
FB	0.00	−0.49	−0.59
NMSE	0.00	0.42	0.53
IA	1.00	0.42	0.59
FAC_2	1.00	0.70	0.57

Note: FAC_2 = factor of two; FB = fractional bias; IA = Index of Agreement; NMSE = Normalized Mean Square Error; R = Pearson's coefficient of Regression; SD = standard deviation.

Table 5. Comparative analysis of model predictions for PM_{10} using nighttime background conditions (10:00 p.m.–6:00 a.m.) from Monitoring Station II for 2016 (Case II)

Statistical parameters	Monitored concentrations	Modeled concentrations (CALINE 4)	Modeled concentrations (STREET) $K=7$
Mean	64	46	42
Systematic bias	—	18	22
SD	17	18	18
R	1.00	0.43	0.45
FB	0.00	−0.32	−0.41
NMSE	0.00	0.22	0.30
IA	1.00	0.58	0.46
FAC_2	1.00	0.86	0.68

Note: FAC_2 = factor of two; FB = fractional bias; IA = Index of Agreement; NMSE = Normalized Mean Square Error; R = Pearson's coefficient of Regression; SD = standard deviation.

there was no movement of any kind near the site, and therefore, was is best suited to act as an actual background site.

Similar to the observation made for Case I, in Case II, the IA values were comparatively higher for STREET (IA = 0.59) than CALINE 4 (IA = 0.42) for 2015 and the reverse was observed for 2016. Similarly, Pearson's correlation coefficient was slightly higher for STREET compared with CALINE 4 for both years. However, the NMSE values were slightly better for CALINE 4 compared with STREET for both years. Further, the monitored concentrations under the present assumption of

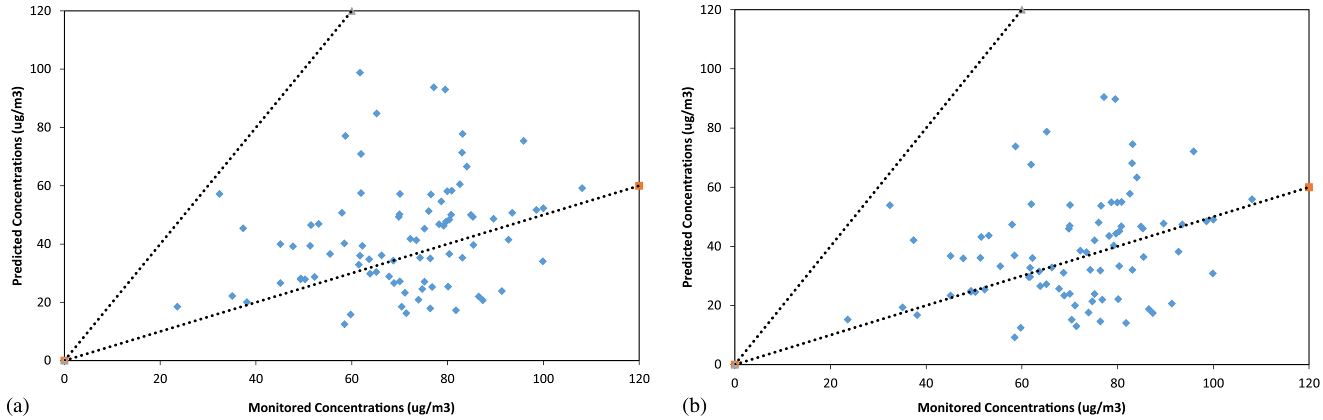

Fig. 3. Scatter plots of modeled and predicted data for PM_{10} using nighttime background conditions (10:00 p.m.–6:00 a.m.) from Monitoring Station II for 2015 (Case II) using: (a) CALINE 4; and (b) STREET.

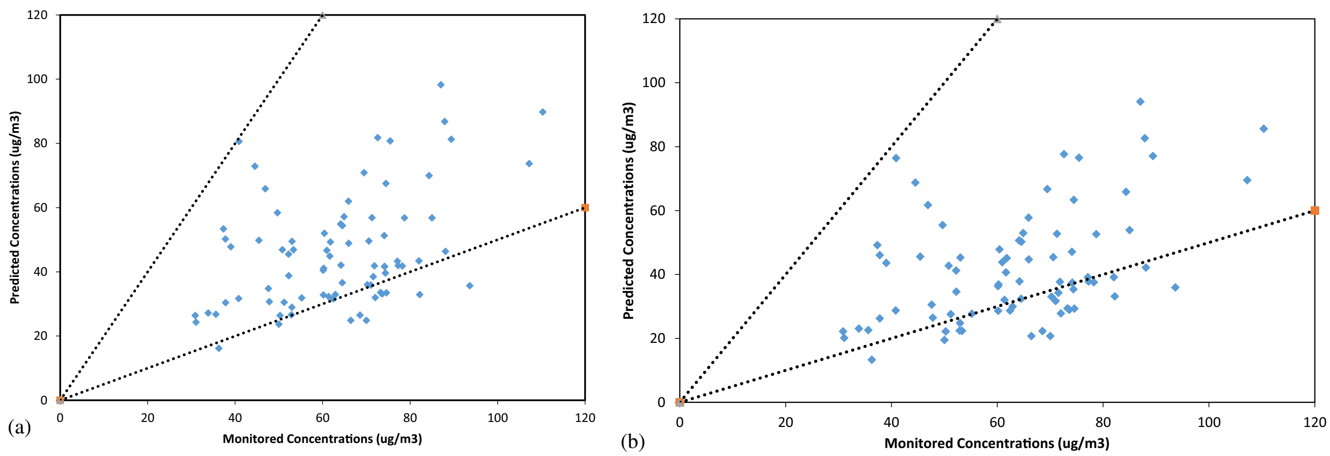

Fig. 4. Scatter plots of modeled and predicted data for PM_{10} using nighttime background conditions (10:00 p.m.–6:00 a.m.) from Monitoring Station II for 2016 (Case II) using: (a) CALINE 4; and (b) STREET.

Table 6. Comparative analysis of model predictions for PM_{10} using nighttime background conditions (10:00 p.m.–6:00 a.m.) from Monitoring Station I for 2015 (Case III)

Statistical parameters	Monitored concentrations	Modeled concentrations (CALINE 4)	Modeled concentrations (STREET) $K = 7$
Mean	70	71	68
Systematic bias	—	−1	2
SD	16	19	19
R	1.00	0.84	0.85
FB	0.00	0.03	−0.02
NMSE	0.00	0.02	0.02
IA	1.00	0.91	0.81
FAC_2	1.00	1.00	0.99

Note: FAC_2 = factor of two; FB = fractional bias; IA = Index of Agreement; NMSE = Normalized Mean Square Error; R = Pearson's coefficient of Regression; SD = standard deviation.

Table 7. Comparative analysis of model predictions for PM_{10} using nighttime background conditions (10:00 p.m.–6:00 a.m.) from Monitoring Station I for 2016 (Case III)

Statistical parameters	Monitored concentrations	Modeled concentrations (CALINE 4)	Modeled concentrations (STREET) $K = 7$
Mean	64	67	62
Systematic bias	—	−3	2
SD	17	22	22
R	1.00	0.80	0.80
FB	0.00	0.05	−0.02
NMSE	0.00	0.05	0.04
IA	1.00	0.86	0.87
FAC_2	1.00	1.00	1.00

Note: FAC_2 = factor of two; FB = fractional bias; IA = Index of Agreement; NMSE = Normalized Mean Square Error; R = Pearson's coefficient of Regression; SD = standard deviation.

background concentrations were 1.4–1.8 times more than the predicted concentrations, which showed severe over predictions. Similarly, the performance of the short-term model parameters varied from model to model and year to year, with long-term model performance being slightly better represented by CALINE 4 than STREET. Finally, it was concluded that the modeling results obtained from the present assumption suggests that Monitoring Station II (which is a designated background site) might not be properly represented as an actual background site.

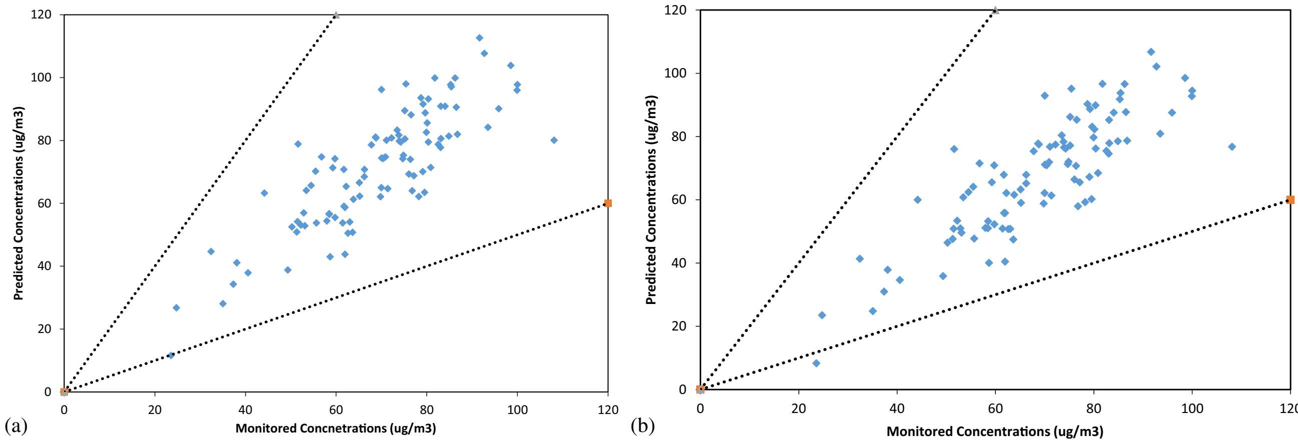

Fig. 5. Scatter plots of modeled and predicted data for PM_{10} using nighttime background conditions (10:00 p.m.–6:00 a.m.) from Monitoring Station I for 2015 (Case III) using: (a) CALINE 4; and (b) STREET.

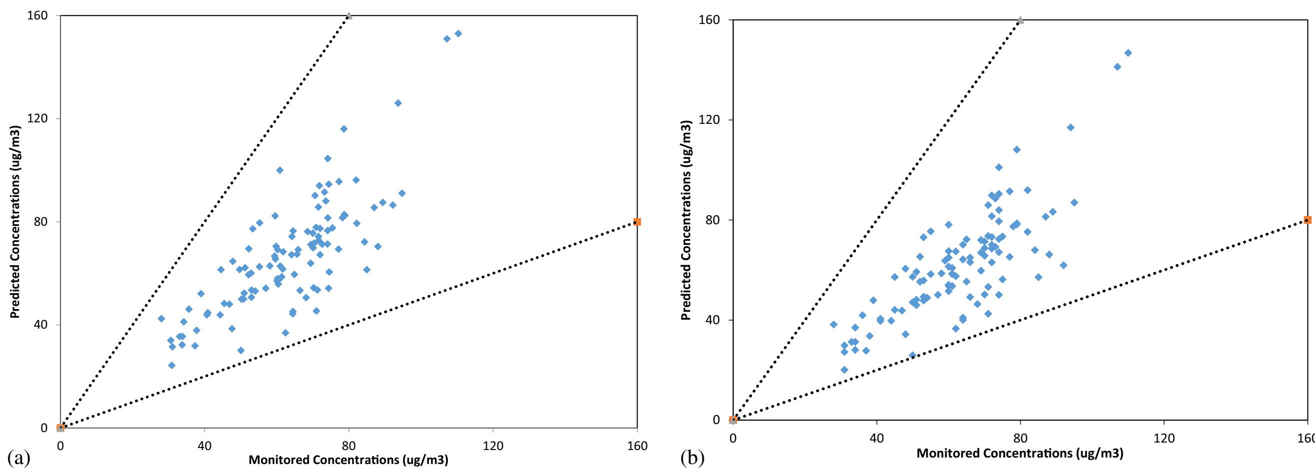

Fig. 6. Scatter plots of modeled and predicted data for PM_{10} using nighttime background conditions (10:00 p.m.–6:00 a.m.) from Monitoring Station I for 2016 (Case III) using: (a) CALINE 4; and (b) STREET.

Modeling Assessment for Case III Conditions

The modeling results obtained using Monitoring Station I as a background site was unsatisfactory and poor even though the site is designated as a background site. Therefore, the modeling analysis was repeated using certain assumptions from the monitoring station itself. Monitoring Station I is a designated urban site. However, the traffic flow decreases significantly in this section between 10:00 p.m. and 6:00 a.m. Hence, the average of the concentrations within this period was considered as the background concentrations. It was observed from the modeling analysis that there was a significant improvement in the modeling results using both the models for both study years. The CALINE 4 model predictions were slightly better for -term model predictions. This is summarized in Tables 6 and 7 and the scatter plots for the monitored and predicted data using the models is shown in Figs. 5 and 6, respectively 2015 and 2016.

Table 8. Comparative analysis of model predictions for PM_{10} using nighttime background conditions (10:00 p.m.–6:00 a.m.) vehicle proportioned from Monitoring Station I for 2015 (Case IV)

Statistical parameters	Monitored concentrations	Modeled concentrations (CALINE 4)	Modeled concentrations (STREET) $K = 7$
Mean	70	59	56
Systematic bias	—	11	14
SD	16	16	15
R	1.00	0.84	0.85
FB	0.00	−0.15	−0.21
NMSE	0.00	0.04	0.07
IA	1.00	0.84	0.79
FAC_2	1.00	0.99	0.99

Note: FAC_2 = factor of two; FB = fractional bias; IA = Index of Agreement; NMSE = Normalized Mean Square Error; R = Pearson's coefficient of Regression; SD = standard deviation.

Modeling Assessment for Case IV Conditions

This assumption builds further on the modeling aspect carried out under the section "Modeling Assessment for Case III Conditions". The assumption in the section "Modeling Assessment for Case III Conditions" suggested that background values would be lowest from 10:00 p.m. to 6:00 a.m. due to the lowest traffic flow (but some traffic flow would be there). Therefore, a 7-day monitoring campaign was carried out from 10:00 p.m. to

6:00 a.m. and the total vehicles were recorded category wise. Thereafter, the emission factors over the sampling period for these vehicles were determined. It was assumed that the ratio obtained between emission factors, which were observed over the sampling period to the overall composite emission factor, would be the contribution due to the traffic flow and the remaining would be attributed to the background factors. The modeling analysis carried out using this scenario is summarized in Tables 8 and 9 and the scatter plots shown in Figs. 7 and 8 for 2015 and 2016, respectively.

Table 9. Comparative analysis of model predictions for PM_{10} using nighttime background conditions (10:00 p.m.–6:00 a.m.) vehicle proportioned from Monitoring Station I for 2016 (Case IV)

Statistical parameters	Monitored concentrations	Modeled concentrations (CALINE 4)	Modeled concentrations (STREET) $K = 7$
Mean	64	56	51
Systematic bias	—	8	13
SD	18	17	18
R	1.00	0.78	0.80
FB	0.00	−0.12	−0.21
NMSE	0.00	0.06	0.08
IA	1.00	0.84	0.80
FAC_2	1.00	0.97	0.97

Note: FAC_2 = factor of two; FB = fractional bias; IA = Index of Agreement; NMSE = Normalized Mean Square Error; R = Pearson's coefficient of Regression; SD = standard deviation.

Discussion on Overall Accuracy of Model Predictions

In an overall context of modeling studies carried out, the results obtained from Cases III and IV led to better model prediction compared with the results obtained from Cases I and II that were based on the actual designated background monitoring station. Some additional details regarding these aspects need to be studied further. In particular, along with probable existing erroneous issues (calibration of the instrument and missing data), there might be some other unknown anthropogenic issues that might affect the recordings at the background monitoring station that needs to be investigated. Further, it is important to note that the nighttime observations during calm conditions might not accurately represent the background concentrations, because the improved ventilation conditions during daytime might mask the effects of vehicular emissions on the observed concentrations. An additional interesting observation from the modeling studies was the consistent underprediction from the STREET model, which is in essence the actual street canyon model compared with CALINE 4. In general, closely spaced buildings with an aspect ratio (H/W) of 0.7

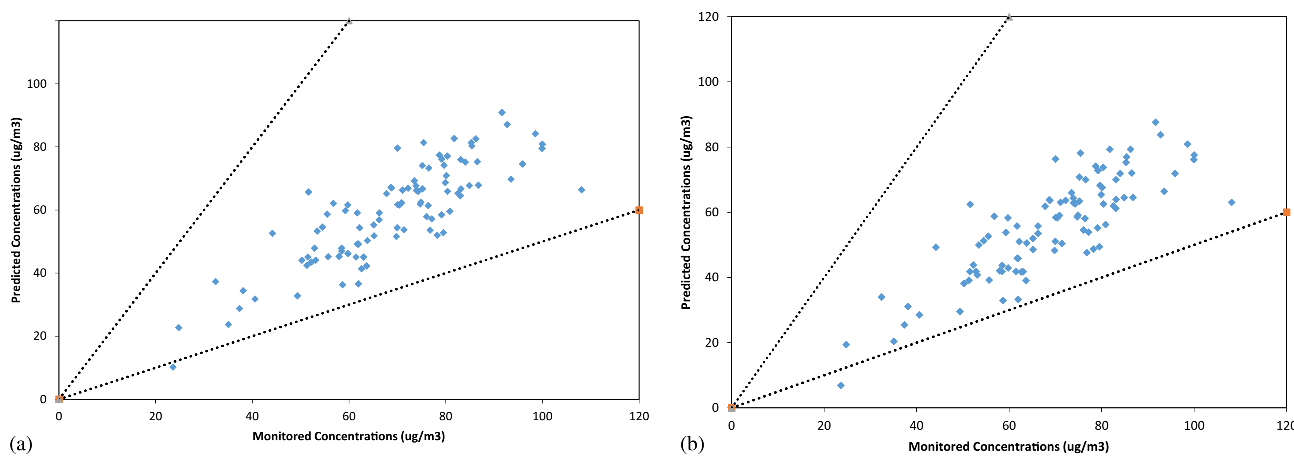

Fig. 7. Scatter plots of modeled and predicted data using CALINE 4 for PM_{10} using nighttime background conditions (10:00 p.m.–6:00 a.m.) vehicle proportioned from Monitoring Station I for 2015 (Case IV) using: (a) CALINE 4; and (b) STREET.

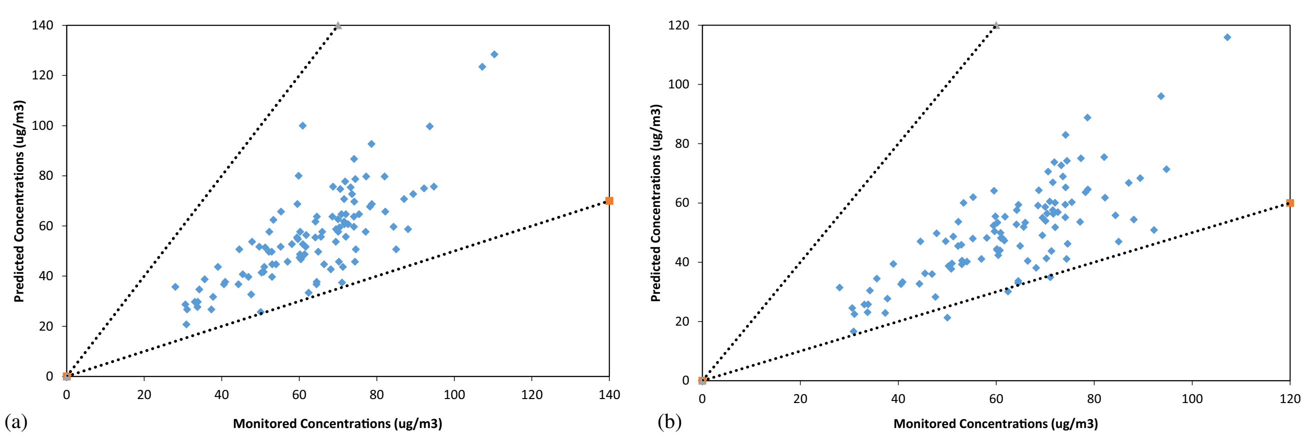

Fig. 8. Scatter plots of modeled and predicted data using CALINE 4 for PM_{10} using nighttime background conditions (10:00 p.m.–6:00 a.m.) vehicle proportioned from Monitoring Station I for 2016 (Case IV) using: (a) CALINE 4; and (b) STREET.

and above results in the formation of circular vortices in the canyon with the ambient flow being decoupled from the street flow. However, despite this study region being an intermediate canyon ($H/W = 1.5$) the wind speed for the majority of time at the location were significantly less and it has been reported that street canyon vortices are not formed at low wind speed conditions (Vardaloukis et al. 2005), which might have affected the model performance of the STREET model.

Limitations of the Study

This study suffers from some inherent limitations. One of the major drawbacks experienced when undertaking the modeling assessment was the lack of basic traffic data. Currently, almost no traffic data is available for the study location (fleet wise classification, yearly wise details, and vehicle flow), which leads to problems in determining the actual composite emission factors. Similarly, since diurnal traffic flow patterns are absent, it was not possible to compute hourly emission factors for use in the modeling studies. Hence, a definitive lack of emission inventory was a major limitation. Another observed issue was that the meteorological data recorded calm conditions for >90% of the study period when modeling was carried out; therefore, the actual number of days modeled for the study period was significantly less and no seasonal variations of the modeling results were presented. Further, from this study, it appears that the background concentrations are not being appropriately recorded by the monitoring station or there might be other local influences that are not being properly represented in the monitored background concentrations. Finally, the preliminary selected models, such as CALINE 4 and STREET require simple input parameters for study; however, even those input values were absent and inherent assumptions were made wherever they were required for a proper assessment of the use of these models. The use of other complex (Gaussian-based) models, such as AERMOD, RLINE, and ADMS would require adequate and appropriate input data before they could be tested for the study location.

Conclusion

The following major conclusions were drawn from the initial modeling studies conducted at the location:

- This study evaluated the performance of the basic air quality dispersion models STREET and CALINE 4 to predict the concentrations of PM_{10} in an urban street in Shimla, India.
- The evaluation was made using four different assumptions of background concentrations. Both of the model predictions were reasonable along the section modeled for the available traffic and meteorological conditions. However, it was observed from the modeling results that background concentrations from the designated site showed poorer results compared with other scenarios considered. It could be possible that background concentrations were not properly recorded or other local influences were affecting the modeling results.
- There is a lack of potential data that could be used as input data for modeling studies including appropriate traffic, meteorological, and background data.
- The PM_{10} concentrations were consistently under-predicted by both the models, but this could be improved with superior urban background measurements and more precise calculation of the emission factors.
- More detailed assessments are required to improve the predictions of the existing air quality in the selected locations of Shimla.

Data Availability Statement

All data, models, and code generated or used during the study appear in the published article.

Supplemental Materials

Figs. S1–S4 are available online in the ASCE Library (www.ascelibrary.org).

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