Available online at www.sciencedirect.com
ScienceDirect
Atmospheric Environment 41 (2007) 7940–7950
ATMOSPHERIC ENVIRONMENT
www.elsevier.com/locate/atmosenv

A semi-empirical box modeling approach for predicting the carbon monoxide concentrations at an urban traffic intersection

Sharad Gokhale[a,*], Suresh Pandian[b]

[a]Department of Civil Engineering, Indian Institute of Technology Guwahati, Guwahati 781 039, India
[b]Center for the Environment, Indian Institute of Technology Guwahati, Guwahati 781 039, India

Received 6 March 2007; received in revised form 16 April 2007; accepted 5 June 2007

Abstract

Emissions generated roadside and at intersections are observed to be affected when there is a sudden change in the traffic flow pattern or increase in the vehicular population, particularly, during peak hours and during special events. The vehicles that queue up at traffic intersections spend a longer amount of time in idle driving mode generating more pollutant emissions per unit time. Other driving patterns (i.e., acceleration, deceleration and cruising) are also observed at intersections, affecting the emission pattern and therefore the resulting pollutant concentrations. The emission rate is not only affected by the increase in the vehicular population but also by the constantly changing traffic flow patterns and vehicles' driving modes. The nature of the vehicle flows also affects the rate and nature of the dispersion of pollutants in the vicinity of the road, influencing the pollutant concentration. It is, therefore, too complex to simulate the effect of such dynamics on the resulting emission rates using conventional deterministic causal models.

In view of this, a simple semi-empirical box model based on the 'traffic flow rate', is demonstrated in the present study for estimating the hourly average carbon monoxide (CO) concentrations on a 1-week data at one of the busiest traffic intersections in Delhi. The index of agreement for a whole week, was found to be 0.84, suggesting that the semi-empirical model is 84% error free. A value of 0.87 was found for weekdays and 0.75 for weekend days. The correlation coefficient for the whole week was found to be 0.75, with 0.78 for the weekdays and 0.62 for the weekend days. The RMSE and RRMSE were found to be 1.87% and 41% for a whole week, with 1.81% and 39.93% for the weekdays and 2.0% and 43.47% for the weekend days, respectively. Specific vehicle emission rates are optimized in this study for individual vehicle category, which may be useful in assessing their impacts on the air quality when there is a significant change in a specific vehicular population and the traffic pattern.

Keywords: Traffic flow rate; Vehicle emission rate; Vehicle density; Semi-empirical box air quality model; Carbon monoxide concentration

1. Introduction

Air quality is poor in many large cities. It tends to be particularly poor at urban traffic intersections and junctions as there is often a sudden change in the traffic flow pattern. Increases in the traffic volume, particularly during peak hours and during

*Corresponding author. Tel.: +91 361 258 2419; fax: +91 361 258 2440.
E-mail address: sharadbg@iitg.ernet.in (S. Gokhale).

1352-2310/$ - see front matter
doi:10.1016/j.atmosenv.2007.06.065

special events, results in higher emissions and higher pollutant concentrations. Vehicles that queue up at an intersection, spend a greater amount of time in idle driving mode generating more pollutant emissions per unit time, often leading to higher pollutant concentrations (Gokhale and Khare, 2004, 2005). Moreover, vehicle driving modes (i.e., idling, accelerating, decelerating and cruising) are variable at intersections which affect the emission pattern and resulting pollutant concentrations. Therefore, the emission rates are not only determined by the vehicular population but also by the traffic flow patterns and driving modes of the vehicles. These are all in constant fluctuation at busy intersections. In addition, the observed concentrations are also affected by the local meteorology (the wind pattern in particular) and the small-scale turbulence created by the vehicles themselves that change depending on the operating mode of the vehicle.

Several air quality models exist for evaluating roadside air quality (Gokhale and Khare, 2004). However, many of the models are too complex to be operated routinely given the simplicity of the available meteorological and traffic data (Dirks et al., 2003). A few models widely used for evaluating the dispersions at roadside, are for example, the GM (Chock, 1978), the GFLSM (Luhar and Patil, 1989), the CALINE-4 (Benson, 1992), the CAR-FMI (Harkonen et al., 1996), and the UCD (Held et al., 2003) models and at street canyons, the OSPM (Berkowicz, 2000; Palmgren et al., 1999) model. Xie et al. (2003) and Vardoulakis et al. (2003) presented a comprehensive review on the models that evaluates the dispersion within the street canyons. These models, which are mainly based on the solutions of complex governing equations, demand more exhaustive inputs to run on an hour-to-hour basis and are computationally complex. In view of this, a trend has now been shifting towards a development of semi-empirical models pertaining to the local conditions. A few researchers have developed such models and applied as alternatives to the rigorous models making use of a priori assumptions about the 'traffic flow' and 'dispersion' conditions (Dirks et al., 2002, 2003; Kassomenos et al., 2004). These models, however, were developed for evaluating the pollutant dispersion in a street canyon and at roadways with a reasonable accuracy in the predictions. There is, however, still a dearth of such models in particular at a traffic intersection wherein vehicle as well as traffic characteristics together generate a complex dispersion phenomenon. The foregoing discussion, therefore, necessitates the need of a simple empirical equation, which can be used to calculate the hourly concentrations based only on the actual 'traffic flow rate' at any site of interests, particularly those at traffic intersections and junctions.

Traffic flow rate is the key to determining the *speed* of traffic (in a congested situation) and the *density* of the traffic flow. The 'vehicle speed' and 'vehicle density' eventually determine the emission rates of the traffic fleet as well as of the individual category vehicles on the road (cars, buses, three-wheelers, two-wheelers, etc.). These variables also change drastically when vehicles approach *intersections* as they experience various driving conditions that affect the emission rates. The usual practice for estimating emissions from vehicles is on the basis of traffic flow modeling, which requires several traffic and vehicle characteristics to be defined quantitatively, in conjunction with a dispersion model to estimate pollutant concentrations from vehicle emissions. Several researchers made an attempt to accurately estimate the emission rates accounting as many features of the vehicles and local conditions as possible by experiment or modeling. For instance, Sturm et al. (2000) and Hausberger et al. (2003) showed that the emission rates measured experimentally from the heavy-duty vehicles were underestimated. Joumard et al. (2000) further showed that the hot emissions under standardized cycle conditions were underestimated by almost 50% for petrol engine cars and 30% for diesel vehicles. Vogel et al. (2000) also found that real-world emissions were much higher than the calculated emissions for CO. In the similar line, Ntziachristos and Samaras (2004) developed speed-dependent emission rates that were compatible with the COPERT-III methodology of emission rates. Gramotnev et al. (2003) also determined the average emission rates for vehicles on a busy road. Most studies are, however, carried out for roadways and, therefore, do not exhibit the realistic speed-dependent emissions which may occur at traffic intersections and junctions.

As an alternative, therefore, a simple semi-empirical box model is developed for a specific traffic intersection on routinely available traffic flow information and meteorological data for predicting an hourly average CO concentration. This modeling approach was proposed by Dirks et al. (2003), which is based on the 'traffic flow rate' and the surface wind speed and direction. This model comprises three components, namely traffic, emission and dispersion. The traffic component of the model requires information on traffic flow rates, jam density and the free-flow speed of vehicles (the speed of vehicles in the absence of any congestion). The emission component of the model uses simple traffic flow theory and empirical relationships as per various drive cycles to estimate the vehicle emission rates (VERs) for vehicle densities ranging from zero (free-flow condition) to the road jam density (completely congested condition). The dispersion component of the model includes a modified empirically optimized box model, requiring wind speed, direction and the vehicle wake factor as inputs.

The present study demonstrates the development and application of the model at one of the busiest traffic intersections in Delhi and presents the results on the CO concentration prediction for a 1-week data of the year 1999.

2. Experimental procedure and data collection

2.1. Site description

The traffic intersection, Income Tax Office (ITO) was selected for the development and the application of the semi-empirical box model. It is one of the most congested intersections in the north part of Delhi city (Fig. 1). It has a number of administrative and commercial buildings, which attract large volume of traffic. The residents surrounding this intersection and the people by virtue of work using this intersection may be exposed to the high levels of CO concentrations (as high as 40% of the hourly observations in a year which exceeded the air quality standard of India for CO, i.e., $4\,\mathrm{mg\,m^{-3}}$). The intersection comprises the major and minor roads crossing each other at right angles, with a separator in the middle of each road. There are two lanes in each direction. The width of each lane is

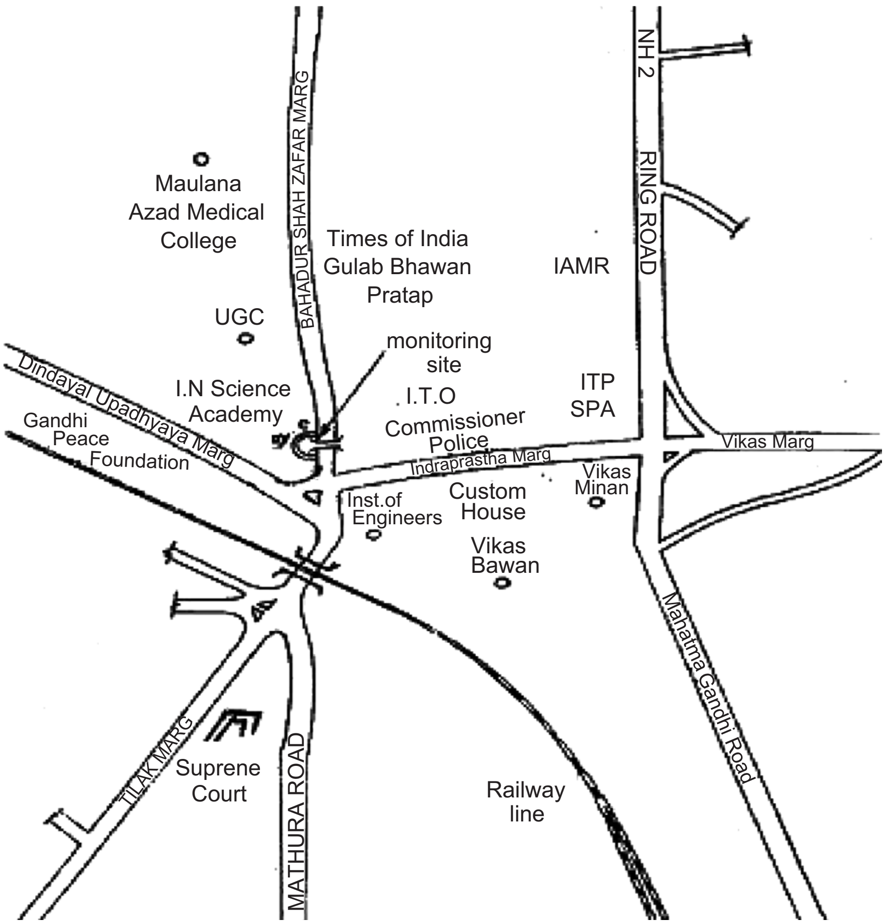

Fig. 1. The ITO traffic intersection with a location of monitoring station.

7.5 m and that of the separator is 1 m. The major road is highly trafficked, while the minor road has traffic almost half of that of the major road. The Central Pollution Control Board (CPCB) maintains a continuous ambient air pollutant monitoring station on the northwest side approximately 18 m away from the center of the major road (2.5 m from the curb of a road) and at a height of 3 m from road level.

Approximately, on the average, 145,000 vehicles (S.D. 26,000) pass through this intersection daily from both directions, with about 8–12% of the total during peak hours (9:00–11:00 h and 17:00–19:00 h) (Gokhale, 2004). About 91% of the fleet consists of light vehicles, (i.e., cars, jeeps, vans), two-wheelers, (i.e., scooters and motorcycles) and three-wheelers, (i.e., auto rickshaws); and about 9% is heavy-duty vehicles (i.e., buses) (CRRI, 1998).

Because of the heavy traffic, a long queue is observed most times of a day, particularly during peak hours, leading to frequent severe traffic congestion. Therefore, free-flow traffic conditions rarely exist at the intersection.

2.2. Traffic data

Traffic count data (i.e., vehicle flows per hour) are important for this study as they are required to estimate the emission rates produced at the intersection. The traffic fleet was classified into four broad categories, viz. diesel-fueled four-wheelers (buses), gasoline-fueled four-wheelers (cars, taxis), three-wheelers (auto rickshaws) and two-wheelers (scooters and motorcycles). Hourly traffic count data were obtained for these four categories of vehicles at the intersection for a period of 1 week for the year 1999, which covered all days of the week including the weekend. The India 2000 mass emission standards equivalent to the Euro-I (also known as EC93, Directives 91/441/EEC, passenger cars only; and 93/59/EEC, passenger cars and light trucks) were adopted in India since the year 2000 for all types of four-wheeled light- and heavy-duty vehicles; however, two- and three-wheeled vehicles continued with the Indian own emission standards. Subsequently, the advanced Euro standards, i.e., Euro-II (EC96), III and IV (EC2004/2005) were implemented in a phased manner following the European Standards as per the Directives 94/12/EC or 96/69/EC and Directive 98/69/EC further amended as 2002/80/EC. Further, the norms for the cars fitted with catalytic converters were introduced in the year 1998. However, the share

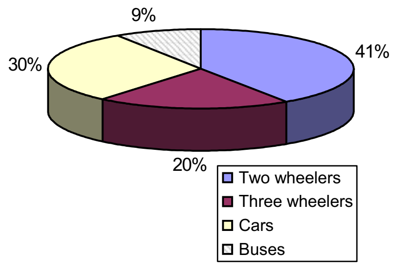

Fig. 2. Percentage composition of traffic (*Source*: CRRI, 1998).

of the petrol-driven cars fitted with catalytic converter was $<5\%$ until the year 1999. It is, therefore, the four-wheeled petrol-driven traffic counts (cars) which are considered to be the non-catalytic type vehicles. Fig. 2 shows the percent composition of the traffic. The jam density[1] is observed to be in the range of 1400 ± 100 of mixed vehicles (traffic fleet). It is found out by actually counting the number of vehicles along the stretch of road leading up to the intersection traffic lights while the vehicles were queued. The maximum free-flow traffic fleet speed (TFS) was observed to be $50\,km\,h^{-1}$, the speed limit of the road.

2.3. Meteorology

The hourly average meteorological parameters such as wind speed, direction and the sunshine hours were obtained from the Indian Meteorological Department, New Delhi, for the year 1999. The hourly stability classes were calculated from the Pasquill–Gifford stability scheme (Schnelle and Dey, 2000) using the solar radiation data in terms of sunshine hours. The wind speed and wind direction, however, serve as the most significant parameters influencing the roadside air quality. It is observed that for most of the time, the wind speed remained $<5\,m\,s^{-1}$ at an anemometer height of 10 m (which measures the threshold value of $0.3\,m\,s^{-1}$ or $1.08\,km\,h^{-1}$); while, 22.5°, the prominent wind direction.

2.4. Carbon monoxide concentration

The 1-hourly average CO concentration data were obtained from CPCB for the year 1999 at the ITO traffic intersection.

[1]Maximum number of mixed vehicles (traffic fleet) occupying the approach road to the intersection in 1 km length near zero flow rate (at which movement of vehicles start ceasing).

3. Modeling methodology

In the present paper, the *traffic component* of the model is developed and evaluated using data collected at the ITO traffic intersection in Delhi. The emission rates in this model are calculated for the traffic fleet as well as for the individual vehicle categories, which allows forecasting the effect of an increase in total traffic flow as well as an individual vehicle category (i.e., car, bus, etc.) at a particular time (peak and slack time) of day on the CO concentration.

The *dispersion component* of the model is developed and evaluated using hourly average wind speed, wind direction-dependent road wind angles, stability-dependent vehicle wake factors and plume height and background concentrations, which are calculated every hour of 1 week from the measured CO concentrations values and the estimated emissions (traffic component) by the semi-empirical model proposed by Dirks et al. (2002).

3.1. Traffic component

This component basically estimates the vehicle density (D, vehicle km^{-1}), as a function of the traffic flow rate (T, vehicle h^{-1}), the jam density (D_j, vehicle km^{-1}) and the maximum free-flow speed of traffic fleet (V_0, km h^{-1}). The relationship between D and T is determined using a standard traffic flow theory (Dirks et al., 2003). The basic assumption of this theory is that vehicles traveling along a road are evenly spaced and traveling at the same vehicle speed (km h^{-1}), i.e., V at a flow rate of T (Eq. (1)). The equations expressing the relationship between D and T as a function of the parameters V_0 and D_j are described as follows (Salter, 1989; Dirks et al., 2003):

$$D = \frac{T}{V}. \tag{1}$$

The relationship between D and V in terms of V_0 and D_j, are represented by

$$V = V_0\left(1 - \frac{D}{D_j}\right). \tag{2}$$

The quadratic relationship obtained by substituting Eq. (1) into Eq. (2) and solving for T is

$$T = DV_0\left(1 - \frac{D}{D_j}\right). \tag{3}$$

D may be calculated for any T by solving Eq. (3) for D as given by

$$D = \frac{D_j}{2}\left(1 \pm \sqrt{1 - \frac{4T}{V_0 D_j}}\right). \tag{4}$$

The negative solution of Eq. (4), which corresponds to the free-flow traffic conditions, is adopted because the vehicle densities remained below the density associated with the maximum traffic flow rate (T_{max}), even during times of peak congestion, as given by

$$D = \frac{D_j}{2}\left(1 - \sqrt{1 - \frac{4T}{V_0 D_j}}\right). \tag{5}$$

To determine the expected T and D for each of the driving conditions considered, i.e., the under

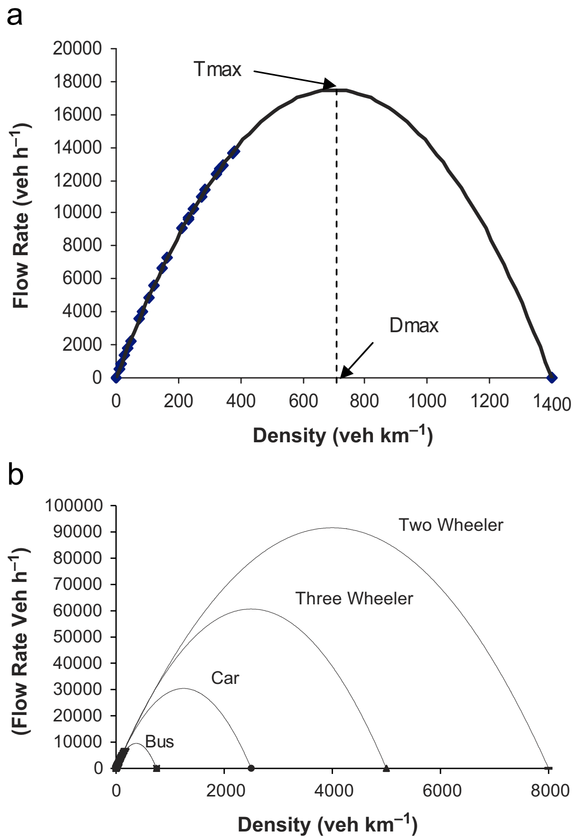

Fig. 3. (a) The relationship between T and D with a V_0 of 50 km h^{-1} and a D_j of 1400 vehicle km^{-1} for the *traffic fleet*; (b) the relationship between T and D with a V_0 of 50 km h^{-1} and a D_j of 750 vehicle km^{-1} for the *buses*, V_0 of 60 km h^{-1} and a D_j of 2500 vehicle km^{-1} for the *cars*, V_0 of 60 km h^{-1} and a D_j of 5000 vehicle km^{-1} for the *three-wheelers*, and V_0 of 75 km h^{-1} and a D_j of 8000 vehicle km^{-1} for the *two-wheelers*.

Table 1
Traffic component parameters for vehicle types

Vehicle type	V_0 (km h^{-1})	Under free-flow condition (km h^{-1})	Interrupted condition (km h^{-1})	Congested condition (km h^{-1})	D_j (vehicle km^{-1})
Cars	60	50	40	20	2500
Buses	50	40	25	10	750
Two-wheelers	75	70	45	25	8000
Three-wheelers	60	50	40	20	5000

free-flow condition, interrupted condition and congested condition, the average TFS, car speed (CS), bus speed (BS), two-wheeler speed (TS) and three-wheeler speed (THS) for each of these driving conditions were obtained by observations by assuming that there were only cars or buses or two-wheelers or three-wheelers.

3.1.1. *Traffic fleet*

The TFS for the under free-flow condition is 40 km h^{-1}, for the interrupted condition is 25 km h^{-1} and for the congested condition is 10 km h^{-1}. The D_j for individual vehicle category was estimated using passenger car unit (PCU) and the capacity of the road length of 1 km. The PCU value for the car was taken as one unit and correspondingly for the two-wheelers was 0.3, for the three-wheelers was 0.5 and for the buses was 3.3. The so-obtained D_j value for the cars was 2500, for the two-wheelers was 8000, for the three-wheelers was 5000 and for the buses was 750. Fig. 3a shows the relationship between the D and the traffic fleet, Tf. It is observed that the traffic flow rate T is well below T_{max} even during the peak hours, which is found to be 17,500 h^{-1} with the corresponding density of 700 vehicles km^{-1} and the speed observed was 25 km h^{-1}. The maximum vehicle density observed is of about 400 vehicle km^{-1}, which is well below the D_{max}. The speed corresponding to the maximum vehicle density is 35.7 km h^{-1}, which is close to the TFS of under free-flow condition. Fig. 3b shows the relationship between the D and the cars fleet, Tc; the buses fleet, Tb; the two-wheelers fleet, T2w and the three-wheelers fleet, T3w. Table 1 describes the traffic component parameters for these vehicle types.

3.2. *Emission component*

Prior to the values of D in Section 3, the relationship between D and VER is obtained using a semi-empirical relation as given in Eq. (6) (Dirks et al., 2003) for all of the vehicle categories. This starts with the estimation of near-zero flow VER_0 for the four driving cycles. The function, in Eq. (6), relates the VER with the D within the range zero to D_j and it varies from VER_0 to infinity, which is a constraint of this equation.

Table 2
Emission component parameters for vehicle types

Vehicle type	VER_0 (g km^{-1} vehicle^{-1})	a	b	c
Traffic fleet	9.11	1×10^{-6}	-4.9×10^{-3}	8.36
Cars	0.56	0.0	2.66×10^{-3}	1.36
Buses	3.20	0.0	1.5×10^{-4}	2.32
Two-wheelers	32.86	0.0	0.22	−73.44
Three-wheelers	0.52	0.0	-2.7×10^{-4}	0.59

$$VER = \frac{(aD^2 + bD + c)D}{D_j - D} + VER_0. \quad (6)$$

The constants a, b and c are determined from the set of VER corresponding to the four driving conditions (maximum free-flow, under free-flow, interrupted and congested). This is done by using the COPERT-III methodology, wherein, the speed-dependent emission rates are estimated for the four categories of the vehicles (COPERT-III (TR-49), 2000). Thus, the VER_0 values were obtained for the traffic fleet as well as for all the vehicle categories. Substituting these values for traffic as well as all vehicle categories, Eq. (6) was evaluated using non-linear regression for the constants a, b and c. The results are shown in Table 2. The negative values of constants may be attributed to the non-linearity that exists in the speed-dependent VER of COPERT-III methodology.

3.2.1. Emission calculations

The emission, Q ($\mathrm{g\,km^{-1}\,s^{-1}}$) for the traffic fleet and the vehicle categories can be calculated using the respective V_0, VER_0, D and D_j (from density-flow rate graphs) and constants a, b and c values as given by Eqs. (7) and (8), respectively,

$$Q = \frac{\mathrm{VER} \times T}{3600} \tag{7}$$

and

$$Q = \sum_{i=\mathrm{car,bus,2w,3w}} \frac{\mathrm{VER}_i \times T_i}{3600}, \tag{8}$$

where i is the individual vehicle category (cars, buses, two-wheelers, three-wheelers). Fig. 4 shows the emission curve (Q) with the traffic flow rate (T). The emission and the vehicle density are multi-valued functions of T, which means the same T corresponds to two D and therefore two Q (Dirks et al., 2003). Each traffic flow rate is therefore characterized by two density values representing different movement speeds. The lower part of the curve, i.e., observed emissions corresponds to the under free-flow condition (i.e., higher speed) and the upper part of the curve corresponds to the congested condition (i.e., lower speed); however, the actual T for the traffic as well as for the vehicle categories observed at the intersection remained well below the maximum possible flow rate.

3.3. Dispersion component

A box model approach is adopted to estimate the dispersions at the traffic intersection. This approach assumes the emissions Q to be mixed uniformly and therefore constant throughout the box and length of the road. The box height refers to the plume height, i.e., Δz (m). The dispersion of pollutants emitted within the box would depend upon the meteorological parameters such as wind speed (i.e., u, $\mathrm{m\,s^{-1}}$) and direction (i.e., θ (in °)) and atmospheric stability (i.e., unstable, neutral and stable), in addition to the value of Δz. However, the mechanical turbulence expressed by the vehicle wake factor (i.e., u_0, $\mathrm{m\,s^{-1}}$), a stability-dependent parameter, proposed by Chock (1978), also avoids the risk of severely over-predicting in very light wind speed conditions. Additionally, the background concentration (i.e., C_b, $\mathrm{mg\,m^{-3}}$) values of the CO are also taken into account and determined empirically. The CO concentration (i.e., C, $\mathrm{mg\,m^{-3}}$) values at the traffic intersection is calculated using Eq. (9), which is based on the equation suggested by Dirks et al. (2003).

$$C = \frac{Q}{\Delta z(u \sin\theta + u_0)} + C_\mathrm{b}. \tag{9}$$

The values of C_b and Δz are estimated by regressing $Q/(u \sin\theta + u_0)$ on C. Here, the 1-hourly average (for a period of 1 week) observed CO concentrations (C), u, θ and u_0 are used for estimating the C_b and Δz. The calculations were done separately for weekdays and weekend days (Saturday and Sunday) as well as for the entire week. To obtain these values, each day (24 data points) was grouped into three sub-groups containing 8 h of values in each sub-group (eight data points) for the whole week (168 data points). The groupings were done based on the period of a day, i.e., early morning time (1:00 to 8:00 h), daytime (9:00 to 16:00 h) and nighttime (17:00 to 00:00 h).

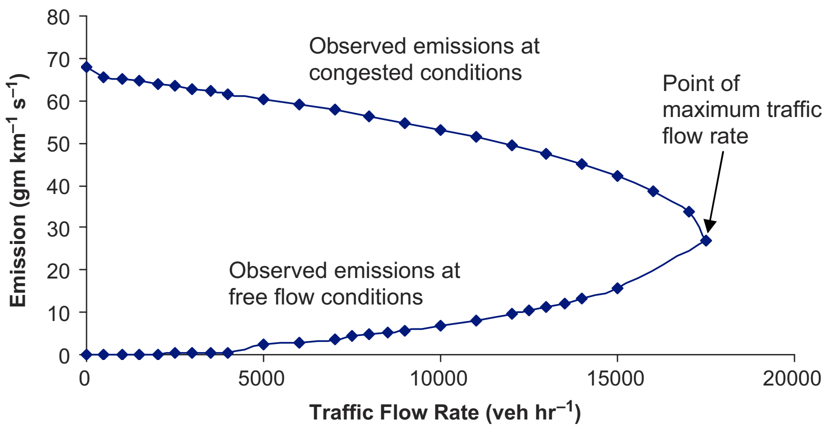

Fig. 4. The effect of T on Q for the *total traffic*.

This was done as the source (traffic) is not dominant in the first group, i.e., during early morning time period; however, significant CO concentrations were observed. This may be attributed to the persistence of CO in the near-field atmosphere during the lean traffic period.

The values of Δz varied between 2.56 and 35.3 m during weekdays and between 3.2 and 11.6 m during the weekend days. The values of C_b were found to be in the range 2.43–12.43 ppm for the entire week with an average value of 4.6 ppm, while, 4.5 ppm for the weekdays and 4.9 ppm for the weekend days.

3.4. Performance evaluation

The performance of the model is evaluated using the correlation coefficient (r) between the observed and predicted concentrations and an index of agreement (d) for weekdays for a week as well as weekend days for a week, in addition to the week as a whole. Additionally, the root mean square error (RMSE) and the relative RMSE (RRMSE) were also used to evaluate the performance of the model. It is observed that the value of r though describes the proportional changes with respect to the means of the two quantities, distinction between the types or magnitudes of variables are not indicated by it, thus, leading to the misinterpretation of the model performance. It was, therefore, Willmot (1982a) suggested using d and RMSE. Several researchers thereafter including Luhar and Patil (1989) and Levitin et al. (2005) used these statistical measures for evaluating the air quality data. The d normally used for the evaluation of air quality data in particular from the vehicles determines the extent to which magnitudes and signs of the observed values about an average measured value are related to the modeled deviation and allows for sensitivity towards the differences in observed and modeled as well as proportionality changes. It varies from 0 to 1, with the value of 1 indicating the model 100% error free, while, the optimum values of the RMSE (expressed in the concentration unit) and the RRMSE (expressed in percentage) are zero. The statistical measures d, RMSE and RRMSE (Oyarzun et al., 2007) are defined in Eqs. (10), (11) and (12), respectively,

$$d = 1 - \frac{\sum (P_i - O_i)^2}{\sum \{|P_i - O_{avg}| + |O_i - O_{avg}|\}^2}, \tag{10}$$

$$\mathrm{RMSE} = \sqrt{\frac{\sum_{i=1}^{n} (P_i - O_i)^2}{n}} \tag{11}$$

and

$$\mathrm{RRMSE} = \frac{\mathrm{RMSE}}{O_{avg}} \times 100, \tag{12}$$

where P_i and O_i are the modeled and observed ith values of CO concentrations, respectively, n is the number of sample and O_{avg} is the mean of measured values.

4. Results and discussion

Fig. 5 shows variation of observed with the predicted CO concentration values. The correlation coefficient, r, for the weekday's data set (Fig. 6a) was found to be 0.78 and 0.62 for the weekend day's data set (Fig. 6b) while it was 0.75 for the whole week (Fig. 6c). The index of agreement d is found to be 0.87 for the weekdays, 0.75 for the weekend days and 0.84 for the whole week. The d values thus explain that the predictions of semi-empirical model developed on a 1-week data are satisfactory and about 84% error free. The RMSE and RRMSE values were found to be 1.87% and 41% for the whole week, 1.81% and 39.93% for the weekdays, and 2.0% and 43.47% for the weekend days, respectively. The RMSE values are (Table 3) found to be reasonably close to the optimum value, while, the RRMSE shows that the magnitude of error in the model prediction is least. The performance of the model was better for the weekdays compared to weekend days, as the predicted values matched well with the observed values. This may be because the higher CO concentrations were observed during weekend days even when the traffic flow rate was low, while during the weekdays. This disproportionate phenomenon may have led to the poor prediction performance for the weekend days. The slight mismatch (i.e., underestimation) may be attributed to the underestimation of the emission rates. The similar studies which are carried out by Dirks et al. (2003) and Kassomenos et al. (2004) also showed the satisfactory results when the semi-empirical model was developed and applied for CO and benzene concentration predictions, respectively.

The reason behind separating the data into weekdays and weekend days is that model can be used to predict the hourly average concentrations during national holidays when significant drop in the vehicular population is observed. However, the

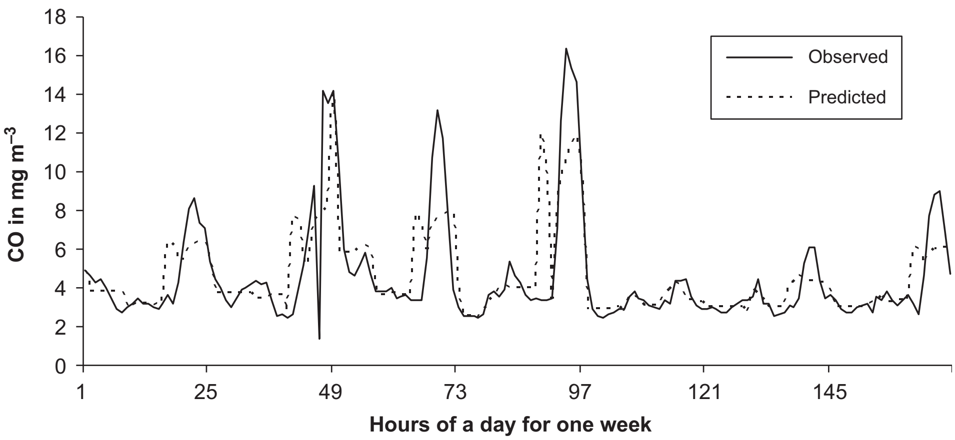

Fig. 5. The comparison of predicted and the observed CO concentration values for a period of 1 week.

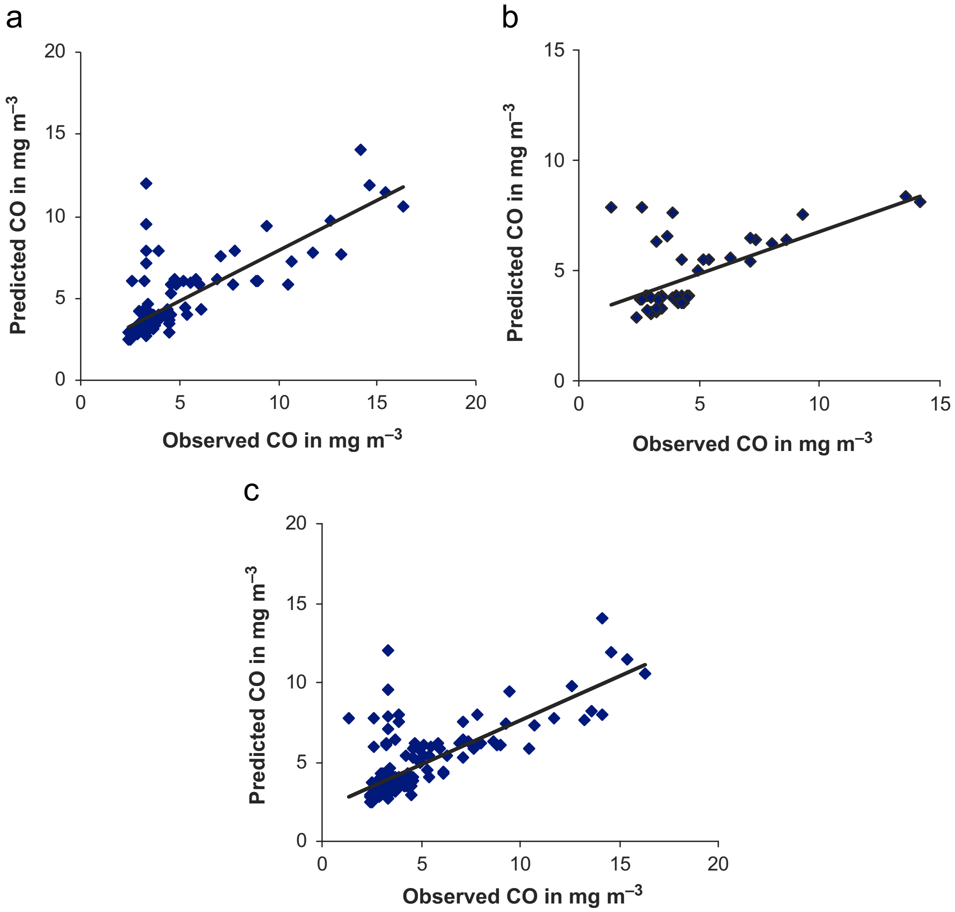

Fig. 6. The scatter plots of the predicted and observed CO concentration values for a data set of (a) weekdays (b) weekend days and (c) whole week.

model's estimated parameters can also be used to predict CO during special congestion hours, which may arise in emergency cases such as construction of flyovers, etc., and similar cases wherein 'what-if scenarios' associated with planned and expected changes in traffic flow patterns (Dirks et al., 2003;

Table 3
Statistical measures for performance evaluation of the model

Statistical measures	For whole week	For weekdays	For weekend days
d (0–1)	0.84	0.86	0.74
r (0–1)	0.75	0.78	0.62
RMSE	1.87	1.81	2.00
RRMSE (%)	41.00	39.93	43.47

Kassomenos et al., 2004). The optimized parameters of the model are also estimated for individual vehicle category. This may be useful in knowing the hourly change in the CO concentration levels due to the variation in the specific vehicle counts in the total traffic. Also there may be a change in the specific vehicle category pattern due to irregular annual growth rate, i.e., the percent rate composition of cars in a total traffic fleet may not remain same every year. For example, there may be a sudden increase in cars and decrease in two-wheelers and yet making the total traffic fleet equal. In such situations, a specific VER for cars and two-wheelers may be used to estimate the impact on the air quality. It is, therefore, the specific information on optimized parameters would be useful in assessing the impacts of the change in the vehicle numbers among the various vehicle categories.

5. Conclusions

This study presented the development and application of a semi-empirical model based on the box approach for the predictions of hourly CO concentrations from the traffic flow pattern which is heterogeneous[2] in nature and a sub-tropical meteorology. In this study, the model is also modified to account for the road wind angles and stability-dependent vehicle wake factors. Since significant changes in the percent distribution of the composition of vehicles are generally observed, an effort was made to develop optimized parameters specific to each vehicle category. The model may, therefore, be utilized to predict the expected concentrations for any hours of a day for any traffic flow patterns and percentage compositions of vehicles.

[2]It is a mixed traffic comprising two-wheelers (scooters, motorcycles), three-wheelers (auto rickshaws), light-duty gasoline-powered (cars, vans, taxis) and light-duty diesel-powered (mini buses, mini trucks) and also non-motorized vehicles, which do not add to emissions but lead to the traffic congestion contributing to vehicle-generated turbulence and ultimately the dispersion of pollutants in the near field of traffic intersections is affected.

Acknowledgements

The authors would like to thank Dr. Kim Dirks for his valuable suggestions in this research.

References

Benson, P.E., 1992. A review of the development and application of the CALINE3 and CALINE4 models. Atmospheric Environment 26B, 379–390.

Berkowicz, R., 2000. OSPM—a parameterised street pollution model. Environmental Monitoring and Assessment 65, 323–331.

Chock, D.P., 1978. A simple line source model for dispersion near roadways. Atmospheric Environment 12, 823–829.

COPERT-III, 2000. Computer programme to calculate emission from road transport, methodology and emission factors, version 2.1. Technical Report No. 49.

CRRI, 1998. Evaluation of emission characteristics and compliance of emission standards for in-use petrol driven vehicles and critical appraisal of the efficacy of the existing pollution checking system in Delhi. Central Road Research Institute, Environment and Road Traffic Safety Division, New Delhi.

Dirks, K.N., Johns, M.D., Hay, J.E., Sturman, A.P., 2002. A simple semi-empirical model for predicting missing carbon monoxide concentrations in records in the absence of emission or traffic data. Atmospheric Environment 36 (39/40), 5953–5959.

Dirks, K.N., Johns, M.D., Hay, J.E., Sturman, A.P., 2003. A semi-empirical model for predicting the effect of changes in traffic flow patterns on carbon monoxide concentrations. Atmospheric Environment 37, 2719–2724.

Gokhale, S., 2004. A hybrid model for prediction of carbon monoxide from vehicular exhausts in urban environments. Ph.D. Thesis, Department of Civil Engineering, Indian Institute of Technology Delhi.

Gokhale, S., Khare, M., 2004. A review of deterministic, stochastic and hybrid vehicular exhausts emission models. International Journal of Transport Management 2 (2), 59–74.

Gokhale, S., Khare, M., 2005. A hybrid model for predicting the carbon monoxide from vehicular exhausts in urban environments. Atmospheric Environment 39 (22), 4025–4040.

Gramotnev, G., Brown, R., Ristovski, Z., Hitchins, J., Morawska, L., 2003. Determination of average emission factors for vehicles on a busy road. Atmospheric Environment 37, 465–474.

Härkönen, J., Valkonen, E., Kukkonen, J., Rantakrans, E., Lahtinen, K., Karppinen, A., Jalkanen L., 1996. A model for the dispersion of pollution from a road network. Finnish Meteorological Institute, Publications on Air Quality, vol. 23, Helsinki, p. 34.

Hausberger, S., Rodler, J., Sturm, P., Rexeis, M., 2003. Emission factors for heavy-duty vehicles and validation by tunnel measurements. Atmospheric Environment 37, 5237–5245.

Held, T., Chang, D.P.Y., Neimeier, D.A., 2003. UCD 2001: an improved model to simulate pollutant dispersion from roadways. Atmospheric Environment 37, 5325–5336.

Joumard, R., Andre, H., Vidon, R., Tassel, P., Pruvost, C., 2000. Influence of driving cycles on unit emissions from passenger cars. Atmospheric Environment 34, 4621–4628.

Kassomenos, P.A., Karakitsios, S.P., Pilidis, G.A., 2004. A simple semi-empirical approach to modeling benzene concentrations in a street canyon. Atmospheric Environment 38, 6073–6078.

Levitin, J., Harkonen, J., Kukkonen, J., Nikmo, J., 2005. Evaluation of the CALINE4 and CAR-FMI models against measurements near a major road. Atmospheric Environment 39, 4439–4452.

Luhar, A.K., Patil, R.S., 1989. A general finite line source model for vehicular pollution prediction. Atmospheric Environment 23 (3), 555–562.

Ntziachristos, L., Samaras, Z., 2004. Speed-dependent representative emission factors for catalyst passenger cars and influencing parameters. Atmospheric Environment 34 (27), 4611–4619.

Oyarzun, R., Arumi, J., Salgado, L., Marino, M., 2007. Sensitivity analysis and field testing of the RISK-N model in the Central Valley of Chile. Agricultural Water Management 87, 251–260.

Palmgren, F., Berkowicz, R., Ziv, A., Hertel, O., 1999. Actual car fleet emissions estimated from urban air quality measurements and street pollution models. Science of the Total Environment 235, 101–109.

Salter, R.J., 1989. Highway Traffic Analysis and Design, second ed. MacMillan, London, pp. 56–60.

Schnelle, K.B., Dey, P.R., 2000. Atmospheric Dispersion Modeling Compliance Guide. McGraw-Hill, New York.

Sturm, P.J., Rodler, J., Lechner, B., Almbauer, R.A., 2000. Validation of emission factors for road vehicles based on street tunnel measurements. International Journal of Vehicle Design 27 (1–4), 65–75.

Vardoulakis, S., Fisherb, B., Pericleousa, K., Gonzalez-Flesca, N., 2003. Modelling air quality in street canyons: a review. Atmospheric Environment 37, 155–182.

Vogel, B., Corsmeier, U., Vogel, H., Fiedler, F., Kulwein, J., Friedrich, R., Obermeier, A., Weppner, J., Kalthoff, N., Baumer, D., Bitzer, A., Jay, K., 2000. Comparison of measured and calculated motorway emission data. Atmospheric Environment 34, 2437–2450.

Willmot, C., 1982a. Some comments on the evaluation of model performance. Bulletin of American Meterological Society 63, 1309–1313.

Xie, S., Zhang, Y., Qi, L., Tang, X., 2003. Spatial distribution of traffic-related pollutant concentrations in street canyons. Atmospheric Environment 37, 3213–3224.