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Validation of Caline 4 Model for Prediction of Carbon Monoxide in the Vicinity of Urban Roads

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ABSTRACT
In order to achieve estimates of urban air quality in the near-field of urban roadways the use of air quality dispersion modeling becomes more significant. In India, CLAINE – 4 has been recommended to predict CO concentration in the proximity of urban roads. Therefore, present study aims at to validate the Caline 4 model for prediction of carbon monoxide in the vicinity of urban roads. The CO monitoring and prediction using Caline – 4 has been carried using real time data. Furthermore, the statistical data analysis for predicted and monitored CO has been carried out to validate the Caline 4 prediction model. The hourly concentration of monitored and predicted CO for both locations clearly shows two peaks (morning and evening) of CO during the day in all the months of the monitoring and prediction. The values of statistical parameters in terms of mean, Index of Agreement (IA), Normalized Mean Square Error (NMSE), Pearson's correlation coefficient (COR), the Fractional Bias and the Factor-of-Two (F2) have been found to be very close to ideal model performance. The values of statistical parameters chosen for the model validation showed good correlation between monitored and predicted values of 1 hourly average CO at both locations of the road.
Keywords: *Urban Roadways, CO Monitoring, CO Prediction, Statistical analysis, Model Validation*

I. INTRODUCTION

Major traffic generated pollutants include CO, NOx and VOC, which consist primarily of hydrocarbons, and particulate matter (PM). All motor vehicles emit CO, but the majority of CO emitted from this source occurs from light-duty, gasoline-powered vehicles. Urban road traffics have been identified as a single major source of air pollution in urban areas (Mukherjee and Viswanathan, 2001) with subsequent adverse human health effects (Chan, *et al.*, 2002; Colvile, *et al.*, 2001). In fact, CO is the result of incomplete fuel combustion that characterize mobile as opposed to stationary pollution sources and therefore, it can be used as an indicator for the contribution of traffic to air pollution (Comrie and Diem, 1999; Heywood,1988). In air quality management, monitoring provides a basis for assessing urban air quality, but it is not possible practically or economically to monitor at every location of interest or predict future levels using this approach alone. Therefore, in order to achieve estimates of air quality on both spatial and temporal scales, the use of air quality dispersion modeling becomes more significant. Several line source models are available to predict pollutant concentrations in the field of urban roadways. But, researchers have used their own countries developed air quality models. However, in India, CLAINE – 4 has been recommended to predict CO concentration in the proximity of urban roads. *CALINE4* is appropriate for nearly all projects involved with roadway and near road emissions. *CALINE4* is capable of specifying links at heights above grade (z = 0), links as bridges (allowing air to flow above and below the link) and links as parking lots (which should be defined by the user as having a height of zero). In addition to evaluating CO and PM dispersion, *CALINE4* incorporates the Discrete Parcel Method for estimating 19 NO2 concentrations. Also, unlike *CAL3QHCR*, *CALINE4* is capable of analyzing the dispersion of pollutants in winds with speeds of less than 1 m/s [Coe, D., et al., 1998]. In addition, Caltrans makes available to users a simplified version of *CALINE4*, known as *CL4*, that includes a user-friendly graphic user interface (Bryan et. al., 2006). Although *CALINE4* also includes a feature for analyzing the effects of nearby canyons or bluffs on pollutant dispersion, it is only recommended for use in rare circumstances and only by very experienced modelers (Bryan et. al., 2006). Chen et al (2008) reported that CALINE4 and CAL3QHC resulted in over-predictions when incremental concentrations due to on-road emission sources were low, while under-predictions occurred when incremental concentrations were high. This model requires large number of input data base such as traffic characteristics (traffic category, traffic volume, traffic speed and emission factor etc.), meteorological parameters (wind speed, wind direction, temperature and atmospheric stability etc.), terrain category (urban, sub urban and rural), and local conditions etc. Therefore, present study aims at to validate the Caline 4 model for prediction of carbon monoxide in the vicinity of urban roads.

II. MATERIALS AND METHOD

The steps of CO monitoring technique, primary and secondary data collection, procedure of their analysis, procedures and steps involved in prediction of CO prediction for the real type parameters using Caline – 4, and statistical analysis of monitored and predicted CO data have been discussed in the subsequent sections. The procedure of statistical data analysis for predicted and monitored CO, comparison of predicted and monitored CO for models validation, and development of linear regression equations for real types of variables have also been discussed herein.

2.1 SITE SELECTION

The sampling points have been fixed at 12 locations of Minto Road for CO Monitoring (Fig. 1) and the real time coordinates of various sampling points have been given in Table 1.

Table 1: Coordinates of sampling locations on Minto Road

S. No.	Sampling Locations	Coordinates			S. No.	Sampling Locations	Coordinates		
		X	Y	Z			X	Y	Z
1	1	20	20	1.8	7	7	20	60	1.8
2	2	0	20	1.8	8	8	0	60	1.8
3	3	-20	20	1.8	9	9	-20	60	1.8
4	4	-20	40	1.8	10	10	-20	80	1.8
5	5	0	40	1.8	11	11	0	80	1.8
6	6	20	40	1.8	12	12	20	80	1.8

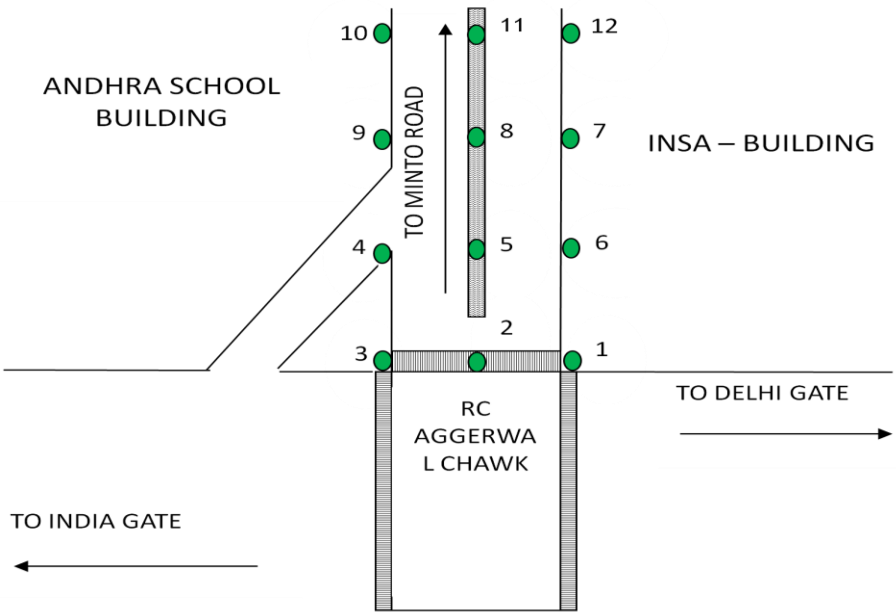

Fig. 1: CO monitoring locations on Minto Road

2.2 PRIMARY AND SECONDARY DATA COLLECTION

The meteorological data including wind speed, wind direction, temperature, atmospheric stability and mixing height have been collected from Meteorological Department of India, Mausam Bhawan, New Delhi – 110003. and CRRI, New Delhi (through personal communication). Furthermore, the representative one day average meteorological data has been evaluated from one month data and used as model input.

2.2.1 Wind Rose Diagram

The collected wind speed and wind direction data have been used to draw wind rose diagram for the month of March, April and May

2011. The monthly wind rose diagram has been drawn using Win-met software. Thereafter, these wind rose diagrams have been used for ascertaining the dominating wind direction. Once dominating wind directions have been ascertained, the location of receptors becomes easier. Fig. 2 shows the wind rose diagram for the month of March, 2011.

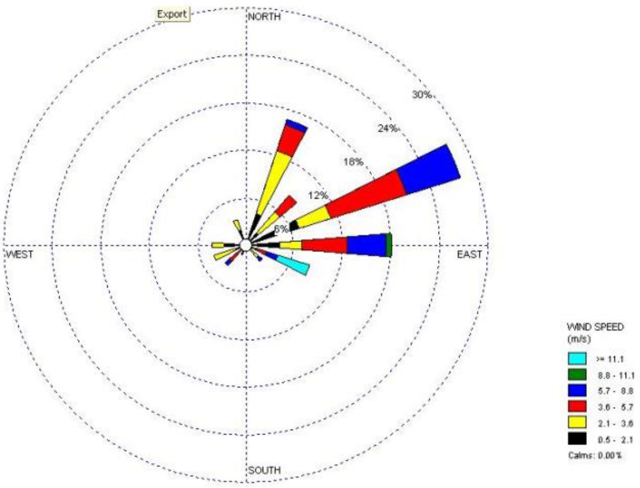

Fig. 2: Wind rose diagram for the month of March, 2011

The wind rose diagram shows dominating wind direction towards South South West to North North East (Broadly West to East) in the month of March.

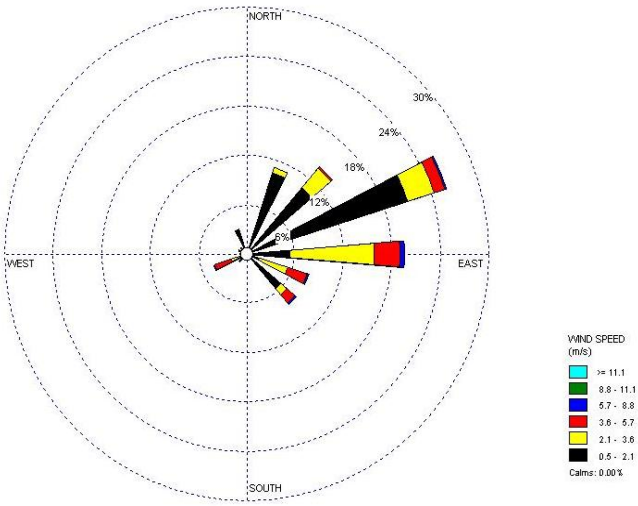

Fig. 3: Wind rose diagram for the month of April, 2011

Fig. 3 shows the wind rose diagram for the month of April, 2011. The wind rose diagram shows dominating wind direction towards South South West to North North East to (Broadly West to East) in the month of April, 2011.

Fig. 4 shows the wind rose diagram for the month of May, 2011. The wind rose diagram shows dominating wind direction towards North North East to South South West (Broadly East to West) in the month of May, 2011.

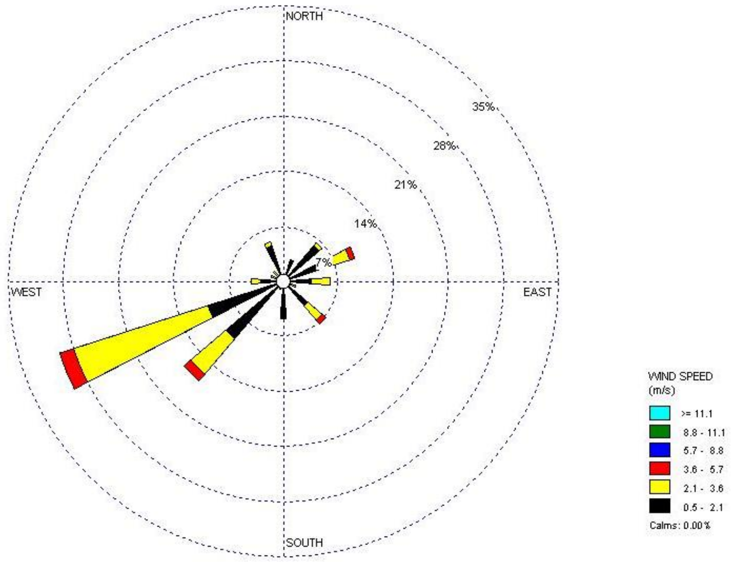

Fig. 4: Wind rose diagram for the month of May, 2011

2.2.2 Collection and Analysis of Traffic Parameters

The traffic volume in terms of vehicles/hour and traffic composition has been collected in the month of March, April and May 2011. The traffic volume comprised of Bus and Trucks (HVs), Light Carriage Vehicles (LCVs), Cars, Three Wheelers (M3W) and Two Wheelers (M2W). The numbers of vehicles have been counted manually at an hourly basis for all the categories. All approach roads - Minto Road side, Delhi Gate side, Laxmi Nagar side and India Gate side have been covered for traffic counts. The traffic counts have been performed from 8:00AM to 8:00 PM continuously. The vintage of vehicles and their corresponding emission factors for different categories of vehicles have been collected published report of CRRI (Central Road Research Institute). The traffic data have been analyzed using MS Excel spread sheet and composite emission factor has been evaluated.

2.2.2 Average Traffic Volume and Composition towards Minto Road side on March, 2011

The hourly traffic volume (vehicles/hr) for different categories of vehicles approaching to Minto Road side has been counted on March 2, 3 and 4, 2011. The three days hourly traffic volume has been averaged and given in Table 3.5. The average traffic volume varied at different hours of the day along with various categories of vehicles.

Table 2: Average hourly traffic volume, vehicles/hr for different categories of vehicles approaching to Minto Road side

Time Period, hrs	HVs	LCVs	CARS	M3W	M2W	Total
8:00 TO 9:00	123	4	1055	456	624	2262
9:00 TO 10:00	144	6	1645	933	1422	4150
10:00 TO 11:00	151	12	1744	1120	1625	4652
11:00 TO 12:00	144	5	1578	986	1754	4467
12:00 TO 13:00	135	8	1365	1109	1801	4418
13:00 TO 14:00	125	12	1416	1324	1624	4501
14:00 TO 15:00	143	9	1533	1345	1466	4496
15:00 TO 16:00	146	10	1389	1142	1352	4039
16:00 TO 17:00	155	13	1347	1025	1651	4191
17:00 TO 18:00	148	8	1522	1129	1709	4516
18:00 TO 19:00	138	9	1501	1011	1560	4219

19:00 TO 20:00	126	5	1423	958	1422	3934

Fig. 5 shows the average traffic volume for the month of March at different hours of the day along with various categories of vehicles. The average heavy vehicles have their maximum numbers (155) at 4:00 PM to 5:00 PM, however, minimum (123) at 8:00 to 9:00 AM. The light carriage vehicles have their maximum numbers (13) at 4:00 PM to 5:00 PM, however, minimum (4) at 8:00 to 9:00 AM. The cars have their maximum numbers (1744) at 10:00 AM to 11:00

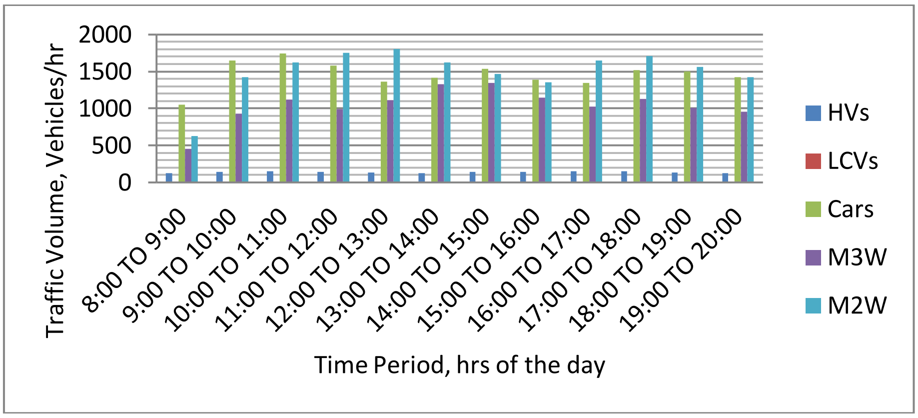

Fig. 5: Average hourly variation of traffic volume at Minto Road side on March, 2011

AM, however, minimum (1055) at 8:00 to 9:00 AM. The Three Wheelers (M3W) have their maximum numbers (1345) at 1:00 PM to 2:00 PM, however, minimum (456) at 8:00 to 9:00 AM. The Two Wheelers (M2W) have their maximum numbers (1801) at 12:00 Noon to 1:00 PM, however, minimum (624) at 8:00 to 9:00 AM.

The Fig. 6 shows the average composition of heavy vehicles (4%), cars (35%), three wheelers (25%) and two wheelers (36%).

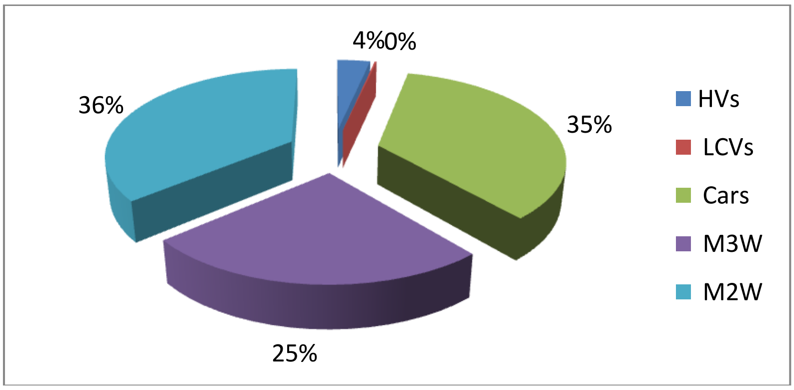

Fig. 6: Average traffic composition at Minto Road on March, 2011

2.3 CO MONITORING PROCEDURE

The CO detector (Model, CO–84) is a portable Carbon Monoxide Detector/ Monitor. In fact, it is a electrochemical cell assembly. A perforated cap at the top end allows the surrounding atmosphere to diffuse in and reach the active part of the cell.

Fig. 7: Portable Carbon Monoxide Detector (Model, CO – 84)

The Carbon Monoxide Detector has been especially designed to detect the CO and indicate its concentration at any time. The CO detector has been described in Fig. 7. This portable Carbon Monoxide Detector has capability to detect the carbon monoxide level from 0.1 ppm to 99 ppm. It does not have any data acquisition system/data storage facility.

The CO concentration has been monitored at selected locations from 8:00 AM to 8:00 PM. CO monitoring has been carried out using portable online CO monitor. Initially, the Instrument has been pre-calibrated and used for CO monitoring at various preselected locations. Since, the instrument did not have data acquisition system/storage system; the data have been manually recorded at 3 minute intervals.

On Minto Road side, the CO Monitoring has been carried out at 12 locations (Location 1 to Location 12) from April 3 to April 18, 2011. At each location, 242 samples have been collected with an interval of 3 minutes. Thereafter, 1 hourly average and 8 hourly average concentration of CO has been evaluated for each location.

2.4 CO PREDICTION PROCEDURE

Prediction of CO concentration at various receptor locations of intersection has been carried out using CALINE-4 model. Initially, relevant information necessary for model run such as traffic volume, composite emission factor and meteorological parameters as well as train conditions have been collected. Thereafter, input files as per model requirement have been prepared and the model run has been performed. The average hourly CO concentration has been obtained at pre-defined receptor locations of the intersection as an output. The CO concentration predictions have been carried out for the months of March, April and May, 2011.

2.5 STATISTICAL ANALYSIS PROCEDURE

Prediction of CO concentration at various receptor locations of intersection has been carried out using CALINE-4 model. Initially, relevant information necessary for model run such as traffic volume, composite emission factor and meteorological parameters as well as train conditions have been collected. Thereafter, input files as per model requirement have been prepared and the model run has been performed. The average hourly CO concentration has been obtained at pre-defined receptor locations of the roadways as an output. The CO concentration predictions have been carried out for the months of March, April and May, 2011.

III. RESULTS AND DISCUSSION

3.1 Comparative Assessment of Monitored and Predicted Results

The predicted hourly concentration of CO at location 4 using Caline – 4 for the month of March shows similar trends of CO concentration variation as discussed in the case of monitored CO concentration (Fig. 8). The values of predicted CO concentrations has been observed to be 3693 µg/m^3 in morning (peak value) followed by evening peak 3924 µg/m^3. It is evident that Caline 4 model under predicted in comparison of monitored values of CO in the month of March. Ganguli et al. (2006) have also reported the under prediction of CO concentration by Caline – 4 and GLSM in their studies.

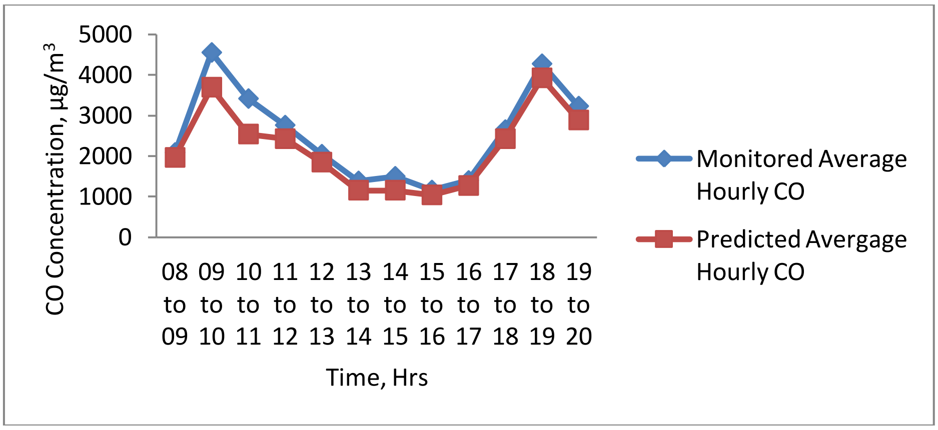

Fig. 8: Comparative monitored and predicted average hourly CO concentration at location 4

The predicted hourly concentration of CO at location 6 using Caline – 4 for the month of March shows similar trends of CO concentration variation as discussed in the case of monitored CO concentration (Fig. 9). The values of predicted CO concentrations has been observed to be (8308 μg/m^3) in morning (peak value) followed by evening peak (7270 μg/m^3). It is evident that Caline 4 model under predicted in comparison of monitored values of CO in the month of March. Ganguli et al. (2006) have also reported the under prediction of CO concentration by Caline – 4 and GLSM in their studies.

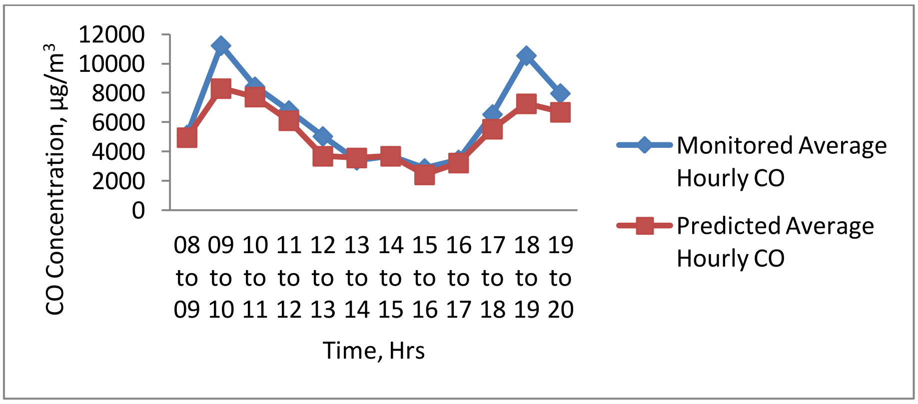

Fig. 9: CEomparative monitored and predicted average hourly CO concentration at location 6

3.2 Caline 4 Model Validation

The values of statistical parameters – mean, Index of Agreement (IA), Normalized Mean Square Error (NMSE), Pearson's Correlation Coefficient (COR), the Fractional Bias and the Factor-of-Two (F2) for monitored and predicted co concentration at Minto Road Side (location 4) have been given in Table 3 and Fig. 10. The value of IA has been found to be 0.95, which is very close to 1.0. This shows perfect agreement between monitored and predicted concentrations of CO. The value of NMSE has been evaluated to be 0.03, which denotes better model performance. The value of Correlation Coefficient, R gives quantitative relation between monitored and predicted results. It has been has been found to be (0.90), close to unity, which implies good model performance. The value of fractional bias (FB) ranges from + 2 to – 2 and has ideal value zero for an ideal.

Table 3: Values of statistical parameters for monitored and predicted concentrations of CO

Parameters	Monitored CO	Predicted CO	Range
Mean	2535	2192	–
Index of Agreement (IA)	1.00	0.95	0.0 – 1.0
NMSE	0.00	0.03	0.0 – 1.0
Pearson's Correlation (R)	1.00	0.90	+ 1 to – 1.0
Fractional Bias (FB)	0.00	-0.11	+ 2 to – 2
F2	100%	86.48	100%

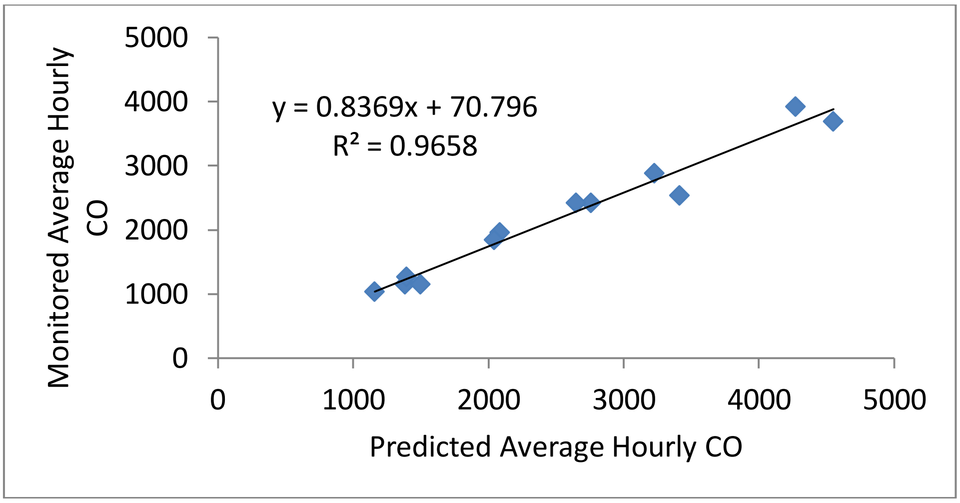

Fig. 10: Correlation between monitored and predicted average hourly CO concentration at location 4

model. The value of FB been evaluated to be – 0.11, which is very close to zero, indicates better performance of model. The ideal value for the Factor-of-Two (F2) should be 1 (100%). The calculated value of F2 has been found to be 86.48%, shows good correlation among monitored and predicted values.

The values of mean, IA, NMSE, R, FB and the F2 for monitored and predicted CO concentration at Minto Road (location 6) have been given in Table 4 and Fig 11. The value of IA has been found to be 0.90, which is very close to 1.0. This shows perfect agreement between monitored and predicted concentrations of CO. The value of NMSE has been evaluated to be 0.06, which denotes better model performance. The value of Correlation Coefficient, R gives quantitative relation between monitored and predicted results. It has been has been found to be (0.88), close to unity, which implies good model performance. The value of fractional bias (FB) ranges from + 2 to – 2 and has ideal value zero for an ideal model. The value of FB been evaluated to be – 0.17, which is very close to zero, indicates better performance of model. The ideal value for the Factor-of-Two (F2) should be 1 (100%). The calculated value of F2 has been found to be 84.12%, shows good correlation among monitored and predicted values.

Table 4: Values of statistical parameters for monitored and predicted concentrations of CO

Parameters	Monitored CO	Predicted CO	Range
Mean	6265	5269	–
Index of Agreement (IA)	1.00	0.90	0.0 – 1.0
NMSE	0.00	0.06	0.0 – 1.0
Pearson’s Correlation (R)	1.00	0.88	+ 1 to – 1.0
Fractional Bias (FB)	0.00	-0.17	+ 2 to – 2
F2	100%	84.12	100%

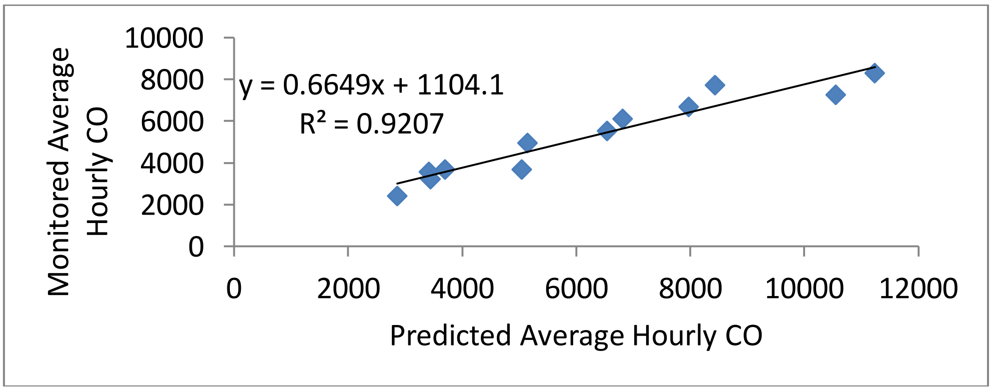

Fig. 11: Correlation between monitored and predicted average hourly CO concentration at location 6

IV. CONCLUSIONS

The comparison of monitored values of average 1 hourly CO concentration levels as well as 8 hourly average concentration levels of CO showed non compliance with the prescribed standards (4000 $\mu g/m^3$ average hourly and 2000 $\mu g/m^3$ average 8 hourly CO concentrations). The hourly concentration of predicted CO for all approach roads clearly shows two peaks (morning and evening) of CO during the day in all the months of the prediction. The predicted values of average hourly concentration CO have been observed to be very close irrespective of location. The values of statistical parameters in terms of mean, Index of Agreement (IA), Normalized Mean Square Error (NMSE), Pearson's correlation coefficient (COR), the Fractional Bias and the Factor-of-Two (F2) have been found to be very close to ideal model performance. The values of statistical parameters chosen for the model validation showed good correlation between monitored and predicted values of 1 hourly average CO at both locations of the road.

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