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# Application of Mathematical Modeling for the Prediction of NOx Concentration due to Vehicular Emission and Model Performance in Gwalior City, (M.P.)

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**Abstract:- Vehicular activities are the major sources of $NO_x$ emissions including other pollutants. Due to hasty growth of vehicles augmented emission levels of pollutants causing severe damage to human health and environment. This paper represents the assessment of $NO_x$ produced by vehicles at traffic rotatory at GoleKaMandir in Gwalior city by using mathematical modeling approach. Mathematical model like General finite line source model (GFLSM) and Delhi finite line source model (DFLSM) are used to assess $NO_x$ level in this study. An emission inventory was prepared for vehicles around the rotatory in three shifts viz. Early morning (EM) (04:00 to 06:00), Morning (MO) (07:00 to 11:00) and Evening (EVE) (07:00 to 11:00). Meteorological data are observed during sampling time at a regular interval of one hour. Predicted data which are simulated by the model and subsequently compared by the observed data of same period were obtained by monitoring through (APM 410) High volume sample. GFLSM holds well with the observed data in comparison to DFLSM as the average value of $NO_x$ (in µg/m$^3$) 33.81 and worked out as, 36.40 and 0.1 through GFLSM and DFLSM. Statistical analysis for the performance of the models reveal GFLSM hold good in comparison to other model with respect to Correlation coefficient (r), Root mean square error (RMSE), and Degree of agreement (d). It is concluded that the levels of $NO_x$ at study area are below NAAQS 2009 norms and GFLSM shows a good response for the prediction of $NO_x$ level in this study area.**

***Keywords*:-** *Vehicular emission, NOx, Emission inventory, Meteorology, Mathematical model, GFLSM, DFLSM, Statistical analysis, Performance Evaluation.*

## I. INTRODUCTION

Due to rapid growth of vehicular traffic in urban areas, vehicular emissions are being produced at high rate day by day which is resulting in degradation of air quality of the cities. Vehicular pollution is one of the major source of pollution in urban areas. The primary pollutants of vehicular emission are$NO_x$ (Oxides of nitrogen), CO (Carbon monoxide), Pb (lead), Particulates matter and HC (Hydrocarbon). Vehicular emissions are considered as a line source of pollutants emission. Automobiles produce $NO_x$ in higher concentration rather than other sources of air pollutants in the city. On the global basis, vehicles contribute about 40%-80% air pollution out of which auto exhaust sources contribute about to 25%-30% $NO_x$ of total anthropogenic emissions (Singh et. al. 2018). Cellular and humoral immune system get affected by the exposure of $NO_x$ (Samet and Utell, 1999). It also affects the lung function causing respiratory problems in long term manner. As per the Indian ground conditions vehicular emission contribution is more, due to poor maintenance of vehicles and poor road pavement quality.

Therefore, it is necessary to formulate, simulate and predict$NO_x$ level in city with due respect to prevailing meteorological conditions. With the introduction of various line source dispersion models likes GFLSM (Luhar and Patil, 1989) and DFLSM (Khare et. al. 1999) etc. simulation of air pollutants along with meteorological conditions can be achieved. This may help in predicting expected levels of pollutants in future enabling authorities to take suitable preventive measures to abate pollution.

A brief study has been done near a traffic rotatory at Golekamandir (GKM) in Gwalior city of Madhya Pradesh, India. The study area is located respectively atlatitude and longitude of 26$^0$13’58.03”N and 78$^0$12’44.04”E respectively. Traffic rotatory of GKM connects two major highway along with the minor routes of city. It is the most busy road intersection within Gwalior city.

Various types of vehicles (ranging from 2-wheeler, 4-wheeler, Buses, Auto, Truck, Tractor-Trailer etc.) passes through rotatory. People living in nearby area are under high pollution risk as it possesses very busy road network, local streets, residential area, industry and institutional building in its nearby locality, Vehicular growth rate observed in Gwalior city is mentioned in a Table1. Data reveals that yearly growth rates of increase in vehicle population falling continuously but number of vehicles are constantly increasing.

| Year | No. Of Vehicles* | Yearly Growth (In %) |
|---|---|---|
| 2013 | 502793 | - |
| 2014 | 555668 | 10.5 |
| 2015 | 601123 | 8.18 |
| 2016 | 651032 | 8.30 |
| 2017 | 683763 | 5.02 |

Table 1:- Yearly growth of registered vehicle in percentage.
*All the data were taken from regional transport authority (RTO).

In Gwalior, limited number of research is carried out related to air pollution in past. This work may be first research work in Gwalior area to address the traffic born air pollution problem by simulation using Mathematical modeling.


Fig 1:- Arial view of study area (Traffic rotatory of GolekaMandir in Gwalior district of Madhya Pradesh.)

## II. METHODS AND MATERIALS

### A. *Emission Inventory*

Descriptive knowledge and accountability of various types of vehicles along with its emissions factor is the basic approach to estimate vehicular air pollution. These factors along with prevailing meteorological conditions and topography helps in working out degree of air pollution likely to be experienced by the community in future (T. Banerjee et. al. 2011). Emissions in the city have been calculated by the emission factor approach for all type of automobile sources which produces emission (Gurjar et. al. 2004). In the present study, $NO_x$source considered as vehicular and it is taken as a line source. The sum of all emission loads due to different kind of vehicles through the study area knowing individual vehicle emission factor may represent the emission rate of any type pollutant due to vehicular emission. Emission load from vehicles has been estimated by using the following equation (Gurjar et. al. 2004, Sindhwani et. al. 2015) (Eqn. (1)).

$$E_i = \sum(Veh_j \times D_j) \times E_{i,j,km} \qquad \text{(Eqn.1)}$$

$E_i$ : Emission due to vehicular activities (kg/hr)
$Veh_j$ : Number of vehicles per type
$D_j$ : Distance traveled in a year per different vehicle type (km/day)
$E_{i,j,km}$ : Emission factor of vehicles (gm/km)

Vehicular count data were obtained by the shift-wise manual survey carried out during study period near the traffic rotatory of GKM area. Numbers of vehicles were counted and categorized like Motor cycles, Auto, Cars, Taxi, Light duty vehicle (LDV) and Heavy duty vehicle (HDV). Emission factor of $NO_x$ for different category of vehicles are taken from previous literature.

| Category Of Vehicle* | Emission Factor For NOx* (gm/km) |
|---|---|
| Motorcycle | 0.03 |
| Auto | 0.1 |
| Cars | 2 |
| Taxi | 0.69 |
| Light Duty Vehicle | 21 |
| Heavy Duty Vehicle | 21 |

Table 2:- Emission factor for vehicle categories.
*Category of vehicle and Emission factor (Gurjar et. al. 2004, T. Banerjee et. al. 2011).

After knowing vehicular count and their respective emission factors for a particular pollutant, it is possible to estimate total emission level of that pollutant due to vehicular activities at study area. Estimated emission levels are then used as input parameter for the prediction of $NO_x$ (Pollutant under consideration) level through mathematical dispersion modeling.

### B. *Micro-Meteorology*

Prevailing meteorological condition influences the emission and dispersion of any chemical species of air pollutant (T. Banerjee et. al. 2011). Meteorological parameters like wind speed, wind-road orientation, and temperature (Singh et. al. 2018) along with cloud cover play an important role in the dispersion of air pollutants. It depend upon the meteorological conditions whether it create a worst condition or a normal condition with respect to building-up of air pollutants as it work as a transporter of the air pollutants. In this study, meteorological data of study area are taken by Accu-weather application during the period of study in which wind speed, wind direction, relative humidity, temperature, pressure and cloud cover are considered. Hourly meteorological data are required as another input parameter in mathematical dispersion model like GFLSM and DFLSM. Apart from this secondary meteorological data like Stability Class, Wind rose diagram were determined by the primary meteorological data as mentioned earlier. For determining stability class and wind rose diagram Pasquill stability class (Turner D.B. 1970, Work book of atmospheric dispersion. *U.S. Environment Protection Agency, AP 26.*) and WR-PLOT (Lake Environment software) were used. Now, the hourly meteorological data of study area act as another input parameter in the mathematical dispersion modeling.

*C. Ambient Air Quality Monitoring (AAQM)*

In this study, a location was selected about 25m away from the center of the traffic rotatory of GKM towards south orientation for setting up an instrument (High volume sampler APM 410, Envirotech, New Delhi, India). Air sampling was done for three days in three shift viz. EM, MO and EVE. $NO_x$ concentration was estimated by laboratory analysis using the modified Jacob and Hochheiser method (IS 5182 part 6, CPCB manual 2013). Sampling was done at a constant flow rate of 1 rpm which creates bubbles in the impinger and sample air is absorbed efficiently by absorbing medium consisting of Sodium hydroxide and Sodium arsenite. $NO_x$ was estimated and the sample was analyzed by using spectrophotometer at a wave length range of 540nm after addition of sulfanilamide, hydrogen peroxide and N-(1-Napthyl)-Ethylenediamine Di-Hydrochloride (NEDA).

*D. Application of Mathematical Model*

Air pollution modeling is a tool to predict or simulate, by physical or numerical means, an ambient concentration of criteria pollutants found in the atmosphere. Dispersion of air pollutant can be explained by a Gaussian model as the dispersion behavior is determined by the standard deviations associated with Gaussian distribution function. These standard deviations are functions of stability class, localized turbulence and downwind distance from the source (Meteorol. Appl. 4, 235-246 (1997)). Gaussian model can be applied on point, area and line source after certain transformation according to the type of source. Gaussian equations (Eqn. 2) for the dispersion of point source are as (RonbanchobApiratikul, 2015)

$$C_{x,y,z,H} = \left[\frac{Q}{2\pi u\sigma_y\sigma_z}\left(\exp\left(\frac{-y^2}{2\sigma_y^2}\right)\right)\left(\exp\left(\frac{-(z-H)^2}{2\sigma_z^2}\right) + \exp\left(\frac{-(z+H)^2}{2\sigma_z^2}\right)\right)\right] \quad \text{(Eqn. 2)}$$

Where,

C = Species concentration at a location x,y,z (gm/m$^3$)
Q = Source emission rate (gm/sec)
U = Average downwind speed normal to the box (m/sec)
$\sigma_y$= Plume dispersion parameter in horizontal crosswind direction (m)
$\sigma_z$= Plume dispersion parameter in vertical crosswind direction (m)
y = Crosswind distance (m)
z = Receptor height above ground (m)
x = Downwind distance (m)
H = Effective source height above the ground (m)

But, for modeling vehicular pollutants in which pollutants are emitted continuously by vehicles, line source models are used (Singh and Gokhale, 2015). For line source following dispersion model like FLSM (Finite line source model), GFLSM, DFLSM, General motor (GM) model, EPA HIWAY, CALINE-3 and AERMOD were used (kumar. A 2016, khareet. al. 1999). In the present study, GFLSM and DFLSM were used as a dispersion model for the prediction of $NO_x$ level at traffic rotator.

➢ *General Finite Line Source Model (GFLSM)*

General finite line source model consider two co-ordinate systems which is wind co-ordinate ($X_1$, $Y_1$, $Z_1$) and the line source co-ordinate (X, Y, Z) along with its transformation (Luhar and Patil, 1989). An equation (Eqn. 3) of GFLSM are as follow (Luhar and Patil, 1989; Khare et. al., 1999; T. Banerjee et. al., 2011; Kumar. A, 2016).

$$C = \frac{Q}{2\sqrt{2\pi\sigma_z u \sin\theta}}\left[e^{\left(\frac{-(z+H)^2}{2\sigma_z^2}\right)} + e^{\left(\frac{-(z-H)^2}{2\sigma_z^2}\right)}\right] \times \left[erf\left(\frac{\sin\theta(p-y)-x\cos\theta}{\sqrt{2\sigma_y}} + erf\left(\frac{\sin\theta(p-y)+x\cos\theta}{\sqrt{2\sigma_y}}\right)\right)\right] \quad \text{(Eqn. 3)}$$

C = Receptor Concentration ($\mu g/m^3$)
Q = Source strength per unit length (gm/m.s)
U = Average wind speed (m/s)
$\theta$= Angle between wind and road varying between 0 and 180$^0$ measured anticlockwise from the road length.
X = Distance from the receptor to the line source (m)
Y = Receptor distance from the roadway center line along the line source (m)
Z = Height of the receptor relative to the ground (m)
H = Effective source height relative to ground (m)
L = Length of the line source (m)
P = Half length of the line source (m, L/2)
$\sigma_y$= Horizontal dispersion coefficients (m)
$\sigma_z$= Vertical dispersion coefficients (m)
erf= Error function,

Error function is described by equation (Eqn 4).

$$erf(x) = \frac{2}{\sqrt{\pi}}\sum_{i=0}^{\alpha}\frac{(-1)^i x^{2i-1}}{i!(2i+1)} \quad \text{(Eqn. 4)}$$

$\sigma_y$&$\sigma_z$can be computed with the help of Pasqulli stability class and Briggs, 1973 equation (Eqn. 5,6)

$$\sigma_y = ax^{0.894} \quad \text{(Eqn. 5)}$$

$$\sigma_z = cx^d + f \quad \text{(Eqn. 6)}$$

The a, c, d and f are constants which is mentioned in a literature (Turner D.B. 1970) and x is a downwind distance in km. $\sigma_y$ and $\sigma_z$ are in meters.

Simplicity of GFLSM makes it popular but it has a limitation of limited receptor co-ordinate to consider. GFLSM also require a condition that the receptor should be located at $90^0$ to the road segment at least three times the distance between the receptor location and road (Ganguly et. al. 2009)

Emission rate computed by emission factor (Gurjar et. al. 2004), meteorological parameter like wind speed, wind direction (in radian) and atmospheric stability (for computing $\sigma_y$ and $\sigma_z$ ) and road characteristic like road geometry and receptor location (x, y, z, $\theta$ ) used as an input parameter for GFLSM.

- *Delhi Finite Line Source Model (DFLSM)*

Study done by M. Khare and P. Sharma over the Delhi traffic conditions at three traffic intersection in Delhi, namely Claridges hotel intersection, Le Meridian intersection, and Hyatt Regency intersection which concluded that GFLSM over predicted as compared to observed data. They found that after elimination of error function in GFLSM performance of model had improved. So they represent a model after elimination of error function in GFLSM as DFLSM according to the Delhi traffic condition.

An equation of DFLSM (Eqn. 7) is as follow (Khare et. al. 1999)

$$C = \frac{Q}{2\sqrt{2\pi\sigma_z u \sin\theta}}\left[e^{\left(\frac{-(z+H)^2}{2\sigma_z^2}\right)} + e^{\left(\frac{-(z-H)^2}{2\sigma_z^2}\right)}\right] \quad \text{(Eqn. 7)}$$

*E. Performance Evaluation of Model*

A performance evaluation of air quality model represents an accuracy of model with respect to its observed and predicted data (Khare et al. 1999; R. sivacoumar et al. 2001; T. Banerjee et al. 2011). A comprehensive package of model evaluation suggested by Juda (1986) which is used for tested monitoring data and predicted data. Willmot and Wicks (1980) suggested using a degree of agreement (d) and root mean square error (RMSE) for the performance evaluation of model.Statistical parameters for the performance evaluation of model (Khare et al. 1999; R. sivacoumar et al. 2001; T. Banerjee et al. 2011) are as follow:

- *Degree of Agreement (d)*

The degree of agreement (d) is expressed in Eqn. 8

$$d = 1 - \left[\frac{\sum_{i=1}^{N}(O_i - P_i)^2}{\sum_{i=1}^{N}(|P_i - \bar{O}| + |O_i - \bar{O}|)^2}\right] = 0 \le d \le 1 \quad \text{(Eqn. 8)}$$

- *Root Mean Square Error (RMSE)*

$$RMSE = \sqrt{\frac{\sum_i^n (O_i - P_i)^2}{N}} \quad \text{(Eqn. 9)}$$

- *Systematic Root Mean Square Error (RMSE$_S$)*

$$RMSE_S = \sqrt{\frac{\sum_i^n [(a + bO_i) - O_i]^2}{N}} \quad \text{(Eqn. 10)}$$

- Unsystematic Root Mean Square Error (RMSE$_u$)

$$RMSE_u = \sqrt{\frac{\sum_i^n [P_i - (a + bO_i)]^2}{N}} \quad \text{(Eqn. 11)}$$

- *Coefficient of Correlation (r)*

$$r = \frac{[\sum_{i=1}^{N}(O_i - \bar{O})(P_i - \bar{P})]}{\sqrt{\sum_{i=1}^{N}(O_i - \bar{O})^2 \sum_{i=1}^{N}(P_i - \bar{P})^2}} \quad \text{(Eqn. 12)}$$

In which a and b are the intercept and slope of regression equation $\overline{P} = a + bO$ ($\overline{P}$ is the mean value of P on a given O) and N is the number of data point.

$$a = \overline{P} - bO \quad \text{(Eqn.13)}$$

$$b = \frac{\left[\left(\sum_{i=1}^{N} O_i P_i - \frac{1}{N}\right) \cdot \sum_{i=1}^{N} O_i \cdot \sum_{i=1}^{N} P_i\right]}{\left[\left(\sum_{i=1}^{N} O_i{}^2 - \frac{1}{N}\right) \cdot \left(\sum_{i=1}^{N} O_i\right)^2\right]} \quad \text{(Eqn. 14)}$$

Both regression coefficients are determined by least square method.If systematic difference tends to zero which represent more accurate model performance. If unsystematic difference tends to RMSE, it represents model is conservative.

## III. RESULT AND DISCUSSION

*A. Emission Inventory*

$NO_x$ were taken as a criteria pollutant among all the air pollutant which is released from the vehicular emission. Data of number of different category vehicle and average travelling of vehicle per day was worked out by conduction of road side survey near the traffic rotatory at GKM. Incorporation of emission factor for $NO_x$ with vehicular activity help in computing emission rate of $NO_x$.

It was found that total emission load of $NO_x$ due to vehicular emission at traffic rotatory of GKM is 53.89 kg/hr. This comprises of emission load of NOx contribution of Motorcycle as 0.14 kg/hr, Auto as 0.22 kg/hr, Cars as 2.80 kg/hr, Taxi as 1.80 kg/hr, LDV as 28.77 kg/hr and HDV as 20.16 kg/hr. Among the different categories of vehicles Light Duty Vehicle has maximum contribution followed by HDV, than Cars, Taxi, Auto and Motorcycle. Traffic rotatory at GKM is a junction of National highway and State highway,

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therefore the movement of LDV and HDV are more frequent at the intersection.

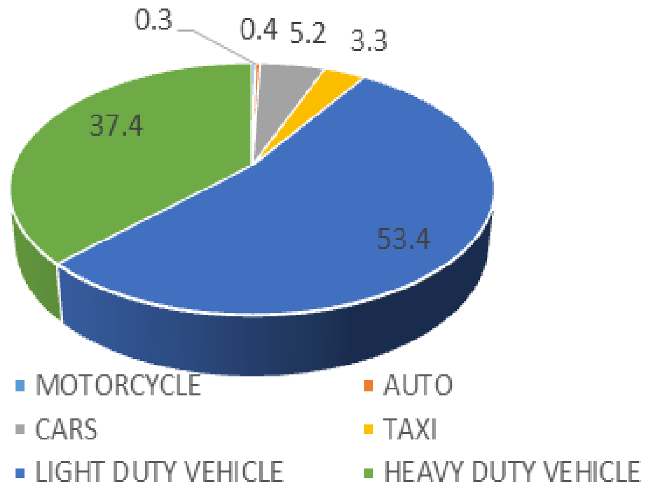


Fig 2:- Percentage contribution of $NO_x$ due to different categories vehicle

*B. Monitoring Data*

Monitoring was done for three days from (30 may to 2 June, 2018) in three shift EM (04:00AM to 06:00AM), MO (07:00AM to 11:00AM), and EVE (07:00PM to 11:00PM) and subsequently laboratory analysis concentration of $NO_x$ was estimated in laboratory.

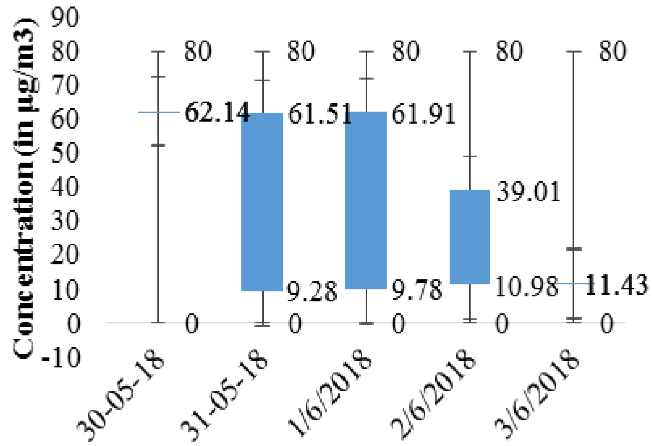


Fig 3:- Temporal variation of ambient $NO_x$ conc. at traffic rotatory of GKM during 30 May 2018 to 3 June 2018.

Total 9 observations were taken at the site 24hr average concentration of $NO_x$ was found to be $33.81\mu g/m^3$ which is less than CPCB standards norms ($80\ \mu g/m^3$). Daily 24hr average concentration of $NO_x$ (in $\mu g/m^3$) observed at site are 62.14, 35.40, 35.11, 25.00 and 11.43 during 30/05/2018 to 03/06/2018 respectively.

*C. Meteorological Parameter*

Meteorological parameter like wind speed, wind direction, temperature and other were taken at an interval of one hour throughout the sampling period. Primary data of meteorology were taken as an input to generate secondary data like stability class and wind rose diagram.

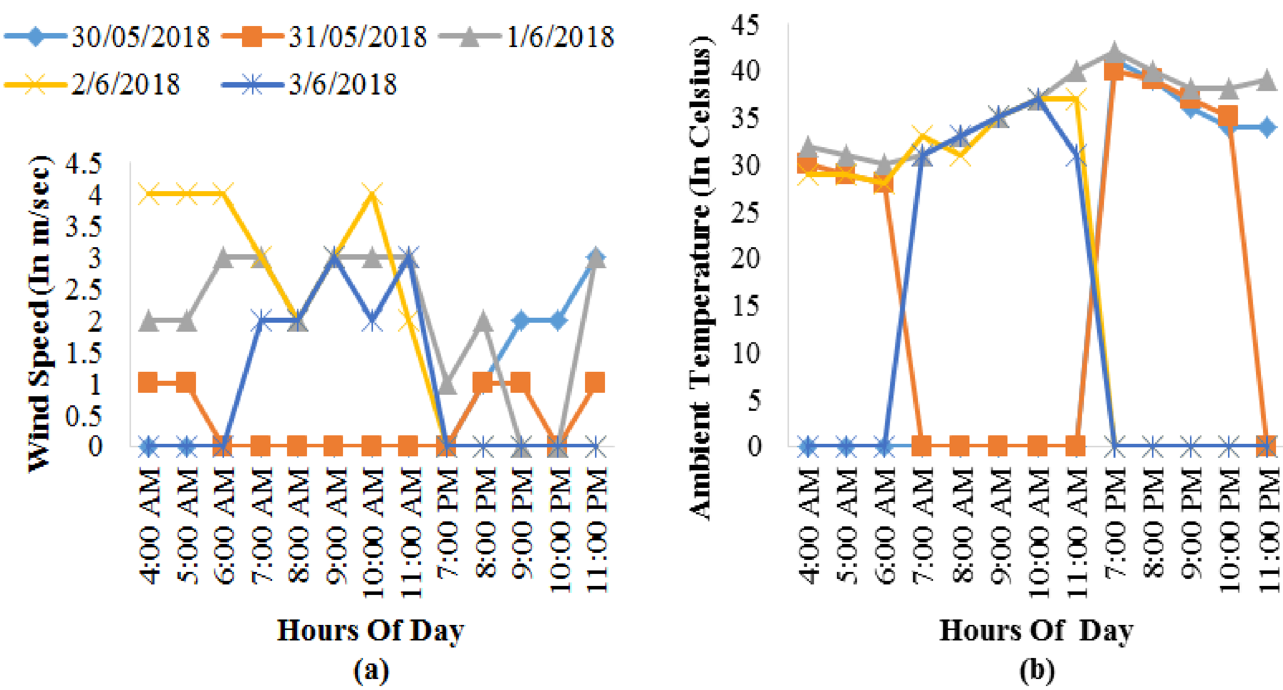


Fig 4:- Diurnal variation of meteorological data (a) Wind speed, (b) Ambient Temperature.

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| S.No. | Date (dd/mm/2018) | Shift | Average Wind Speed (In M/S) | Stability Class | Stability Condition |
|---|---|---|---|---|---|
| 1 | 30/05 | EVE | 1.6 | F | Moderately stable |
| 2 | 31/05 | EM | 0.67 | B | Moderately unstable |
| 3 | | EVE | 0.50 | D | Neutral |
| 4 | 1/6 | EM | 2.33 | C | Slightly unstable |
| 5 | | MO | 2.80 | A | Strongly unstable |
| 6 | | EVE | 1.20 | F | Moderately stable |
| 7 | 2/6 | EM | 4.00 | D | Neutral |
| 8 | | MO | 2.80 | A | Strongly unstable |
| 9 | 3/6 | MO | 2.40 | A | Strongly unstable |

Table 3:- Diurnal shift-wise average wind speed and stability class.

WR-PLOT software of Lake Environment were used for plotting wind rose diagram which are shown in a fig.5 (a-e)

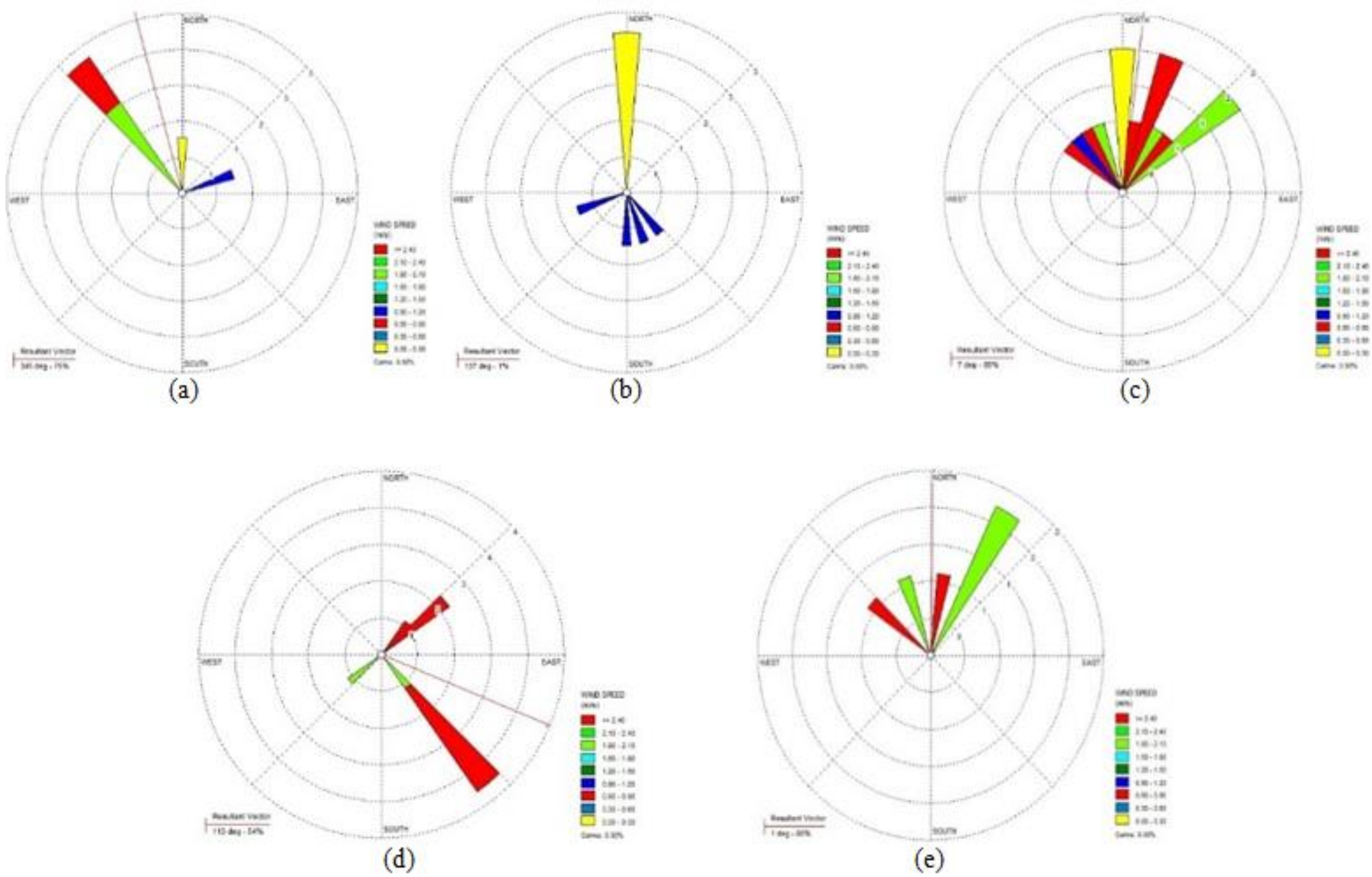


Fig 5:- Wind rose diagram (a) 30/05 (b) 31/05 (c) 01/06 (d) 02/06 (e) 03/06

*D. Interpretation of GFLSM and DFLSM Prediction*

GFLSM simulation was done along with the input parameter of road characteristic and meteorological parameter which shows a better result in comparison of DFLSM with respect to AAQ monitored data. As the average value of $NO_x$ concentration (in $\mu g/m^3$) through AAQ monitored data, GFLSM and DFLSM worked out as 33.81, 36.40 and 0.1 respectively. DFLSM does not hold well according to the condition of study area. Results shows GFLSM can be used as suitable model for the prediction of $NO_x$ concentration as its outcomes are very close to the observed values.

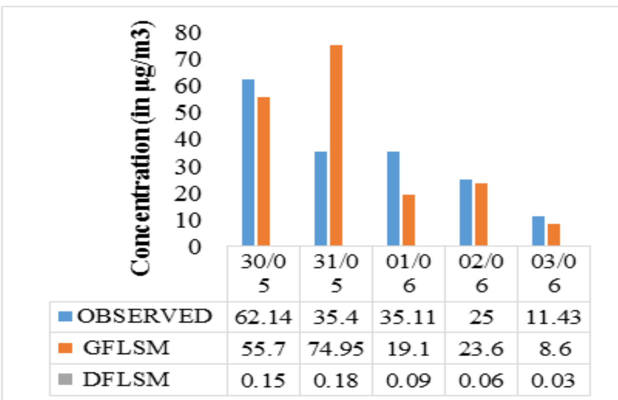


**Fig.6.** Graph shows a comparison between observed and predicted data.

*E. Statistical Analysis*

Performance of GFLSM was found good as their result lies near the ideal value of various statistical parameters. Final outcome of the statistical analysis indicates that the accuracy of the GFLSM and DFLSM were 80% and 46% approximately. Other statistical parameter observation results are shown in Table 4

| S.No. | Parameter | Unit | Perfect Model | GFLSM | DFLSM |
|---|---|---|---|---|---|
| 1 | RMSE | $\mu g/m^3$ | - | 24.45 | 40.10 |
| 2 | $RMSE_S$ | $\mu g/m^3$ | 0.0 | 4.41 | 40.15 |
| 3 | $RMSE_U$ | $\mu g/m^3$ | RMSE | 24.04 | 0.08 |
| 4 | Correlation coefficient (r) | - | 1.0 | 0.74 | 0.87 |
| 5 | Degree of agreement (d) | % | 100 | 80 | 46 |

Table 4:- Statistical parameter analysis result

Although, It is found that GFLSM have correlation coefficient value (as shown in figure 7 (a, b)) less than DFLSM but it may be considered satisfactory. In case of other parameters GFLSM holds well in comparison of DFLSM excluding its coefficient of correlation. So the overall statistical analysis favors GFLSM to be used as substitute tool for the prediction of $NO_x$ concentration at traffic rotatory in GKM due to vehicular emission.

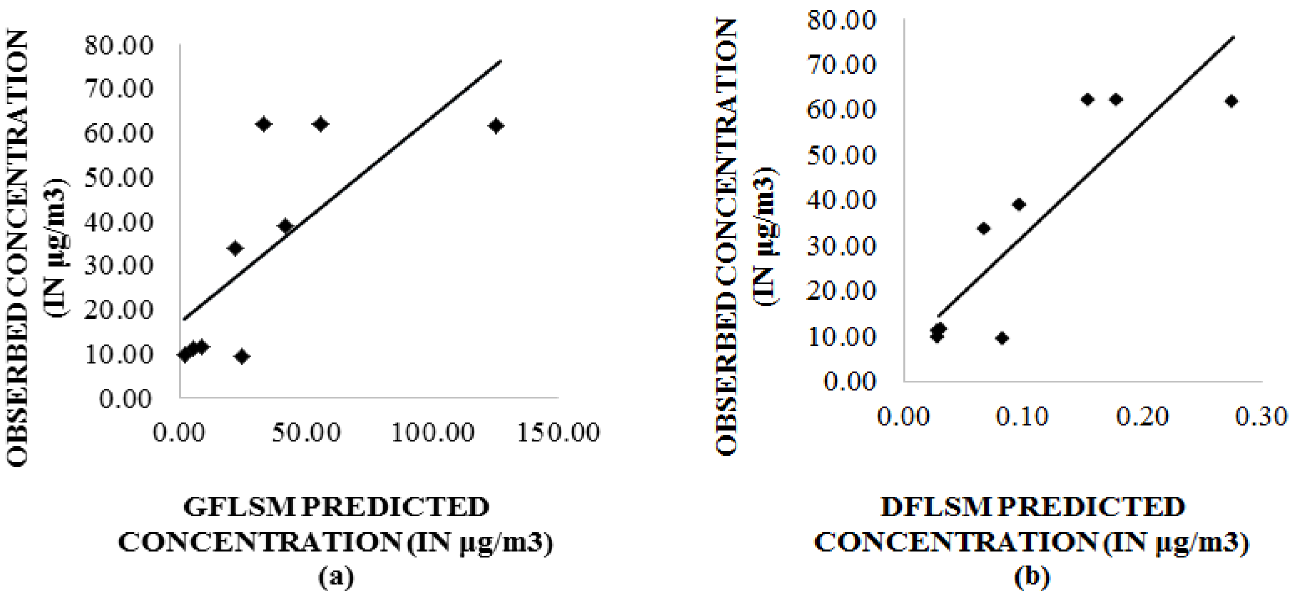


Fig 7:- Correlation between monitoring data and (a) Predicted data by GFLSM (b) Predicted data by DFLSM.

## IV. CONCLUSION

A comprehensive study of application of mathematical modeling for predicting $NO_x$ concentration due to vehicular emission on traffic rotatory at GKM, Gwalior city is reported. Emission inventory of vehicle has done during study period to reveals that total emission load of $NO_x$ is 53.89 kg/hr out of which Light Duty vehicle shows highest contribution of 28.77 kg/hr (53.4 % of total emission load). Further, monitoring data show that the 24hr averaged concentration of $NO_x$at GKM rotatory during sampling period was 33.81 $\mu g/m^3$which is below the standard norms given by CPCB for NOx (80 $\mu g/m^3$). This represents a lower level of $NO_x$ in the study area. Mathematical modeling through GFLSM, predicted 24 hr averaged concentration of NOx was 36.40 $\mu g/m^3$ which reveals the suitability of GFLSM because of higher level of confidence prevails in GFLSM in comparison of DFLSM. Statistical analysis revels about the performance of model in which GFLSM show its applicability approximately 80%. Conclusively, it may be stated that GFLSM will also give better result for prediction of air pollutants due to traffic near other traffic rotatory in the Gwalior city due to vehicular emission.There is a further scope for other researcher to do an assessment of air pollutant due to vehicular emission with the application of GFLSM for forecasting of NOx concentration as other important areas and strategic locations in Gwalior.

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