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Modelling and Simulation of Ambient Carbon Monoxide

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Abstract Air pollution affects both the health and environment of living organisms. In large urban cities the emissions of carbon monoxide (CO) gas from the transport sector pose unprecedented risks being a silent and lethal killer. In order to eradicate the adverse impact of CO pollution, there exists a need for an early warning system, which may be of immense help to manage and regulate ambient CO concentrations. CO emission and its dispersion is a non-linear problem which can be vividly expressed using artificial neural network (ANN) computations. In this paper an attempt is made to simulate concentration of CO gas based on historical data using ANN. Eleven years (1996-2006), morning time (06.00hrs-14.00hrs) CO emission data from ITO square of Delhi has been employed for modelling and simulation. The ANN are regarded as an efficient and optimised architectures for capturing the inherited codes of processes and technique for estimation as compare traditional statistical techniques. The modelling result shows comparable matching with the measured ambient values of CO.

KEYWORDS:- Simulation , Modelling , Concentration, Artificial Neural Network (ANN), Real time analysis

I. INTRODUCTION

Atmospheric pollutants are responsible for both acute and chronic effects on human health (WHO, 2000). Air pollution is a major environmental concern, affecting environment of peoples and properties.. Enhanced exploitive use of natural energy resources has resulted in rising emission of potentially harmful gases and particulate matters into the atmosphere. In urban areas vehicular emissions (e.g. Carbon monoxide (CO), nitrogen oxides (NOx), hydrocarbons, particulate matters and sulphur oxides (SOx)) have been recognized as the major sources of air pollution. Over the last three decades, motor vehicle numbers have been doubling every 10 or fewer years in many Asian countries, as against a 2–5% annual growth rate in Developed Countries [1]. Being the prime end product of vehicular emission the CO gas has emerged as main polluting gas amounting approximately 70% contribution through transport sector only [2]. According to Davis and Cornwell [3] carbon monoxide is a colourless, odourless, tasteless and non-irritating gas that can be lethal to human beings within minutes at high concentrations exceeding 12,800 parts per million (ppm). In urban environments and especially in those areas where population and traffic density are relatively high, human exposure to hazardous substances is expected to be significantly increased. This is often the case near busy traffic points in city center, where urban situation may contribute to the creation of poor air dispersion conditions giving rise to contamination hotspots [4]. The contributions of various sources of air pollution in the ambient air of Delhi are listed in Table I.

Table I-Trends in the Contribution of Pollution Sources

SN	Source	1970-79	1980-89	1990-99	2000-09	2010-
1	Industrial	56%	40%	29%	20%	20%
2	Vehicular	23%	42%	64%	72%	74%
3	Domestic	21%	18%	7%	8%	6%

Emission load of CO in Delhi (422 MT/day in the year 2002) has been much greater than the other air pollutants and in other metros in India. It is due to cumulative effects of population growth, industrialization and increased vehicular use.

Due to increasing vehicular air pollution in Delhi a series of policy measures have been undertaken over the last decade to address the increasing vehicular air pollution problems in Delhi and other Indian mega cities, but without any effective improvements in the urban environment. Hence, it needs an integrated and efficient approach to address the fundamental problems of urban air pollution and provide a basis for future regional cooperation. This may be best done using pre-warning (forecasting) system based on the modeling and simulating the past realizations of air pollution data. In the present study an ANN model is developed to forecast emission of CO gas.

A. Air Quality Modeling Review

Air quality modeling (AQM) helps to predict the time ahead concentration of pollutant and thus assist to assess the impact of any proposed project on air environment and simultaneously analyses the travel behavioral strategies to mitigate possible negative impacts. Many AQM models have been developed to forecast CO concentration and health effect. These CO forecast models can be broadly classified into six major categories, viz. statistical, deterministic, numerical, stochastic, soft computing and hybrid [5] Tanaka et al., (1992) [6] first attempted neural network and fuzzy methods for the identification and analysis of suitable forecasting model for CO concentration and used self learning approach for it. Later the work has been extended for modeling and control of non linear CO concentration series [7]. Moseholm et al. (1996) [8] studied the usefulness of neural network to understand the relationships between traffic parameters and CO concentrations measured near an road intersection. Dorzdowicz et al.

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(1997) [9] developed a dispersion model based on neural network to estimate hourly mean concentrations of CO in the urban area of Rosario City, Argentina. Gardner et al. (1999) [10] developed a multilayer perception NN model to estimate hourly NO_x concentrations using meteorological data of Central London, showing that the ANN outperformed the ordinary least squared model.

In recent years, the considerable progress has been in the developing of neural network (NN) models for air quality forecasting [11],[12]. Nagendra and Khare (2002) [13] presented a detailed review of vehicular exhaust emission models including ANN based models. Nagendra and Khare (2002, 2003 and 2004) developed an ANN-based line source model to forecast CO concentrations wicomparisons of numerical results with observed data in an intersection and a link. Zhang et al., (2004) [14], studied relation between Traffic emission and vehicle parameter using Image processing and remote sensing techniques.

Furthermore, Grivas et al. (2006) [15] used neural networks to predict PM_{10} hourly concentrations in the metropolitan area of Athens, comparing their performance with a multivariate regression model, whereas Pelliccioni et al. (2006) [16] showed that the integrated use of dispersion models and neural networks can improve the prediction performance. Yang et al., (2007) [17], presented an ANN technique to forecast real time short cut roadside CO and CO_2 concentrations, considering the effects of traffic flow and road conditions.

B. Description of the Study Area and Data

India's National Capital Region (NCR) informally known as Delhi city is situated at **Latitude**: +28.67 (28°40'12"N) and **Longitude**: +77.21 (77°12'36"E) with **Time zone**: UTC+5:30 hours (i.e. **Local time**: 14:50:06) is a highly urbanised city supporting about 16.7 million people living in a dense manner (population density of 11320 person / sq km according to the year 2011 Census). The ITO crossing (core zone) is the busiest traffic intersection of Delhi having the biggest commercial area, has been selected for the study. The majority of vehicles comprise petrol driven 2 and 3 wheelers, cars and buses. The area comprises typical topographical features with residential cum commercial complexes & traffic routes, surrounded by industries, agricultural land, and Yamuna river (the sink) etc. The area have the Av. Vehicle Density = 14275 pcu, with Av. Pollution Load (in terms of CO) = 0.4 g/s-m^2. ITO junction falls under category of heavy Traffic zone, having seven lanes and medians. The ITO intersections handle the maximum peak hour bus traffic on the corridor which exceeds 600 buses per hour per direction.

The CO monitoring data at ITO crossing of Delhi is collected from the CPCB (2008) New Delhi, India, and is to used in this study. Morning time (06.00hrs-14.00hrs) data of CO gas has been simulated using ANN modeling to generate forecast.

II. METHODOLOGY

The forecasting hot spot air quality and specifically high pollution episodes in urban air are recent requirements of air quality research [18]. An artificial neural network (ANNs) is a quite efficient tool for modelling and Simulating CO air pollution time series with less effort, provided that efficient architectures are available. ANN is special Kind of Intelligent Systems whose computing power is achieved through their massively parallel distributed structure and their ability to learn and therefore generalize. An ANN is considered successful only when it proves its ability to generalize. Generalization is a measure of an ANN's ability to produce reasonable output for inputs those are not encountered during the training phase [19]. Due to their ability to learn from input data either in supervised or in unsupervised mode, the ANN is used in many applications of engineering, mathematics, physics, neurosciences and statistics.

A neural network is a distributed computational system with a number of individual, and interconnected artificial neurons (variously referred to as "Processing elements" (E1, E2…..), "Nodes", or "Units") which have several input paths (input and hidden layers) and one output path (layer). These neurons are located in one of three types of layers: the input layer, the hidden layer, or the output layer Fig. (1).

The input neurons receive data from the outside environment, the hidden neurons receive signals from all of the neurons in the preceding layer, and the output neurons send information back to the external environment. The neurons use various rules that combines the input signals and an activation rule that processes the combined signal and calculates the output [20]. Neural net operates in some specific predefined architecture, and could be trained to self-modify connection strengths during the processing (learning) of element parameters [19].

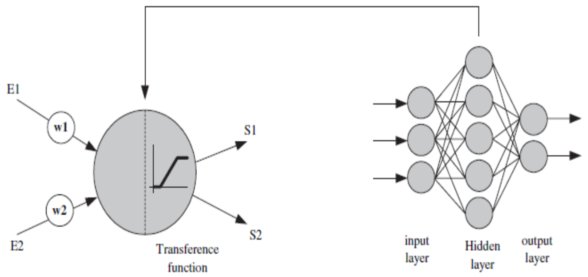

Figure (1): Artificial Neural Network Structure

Stanley (1990) [21] indicated that the way in which the neurons are connected to each other in a network typology has a great effect on the operation and performance of the network. Accordingly, ANN models come in a variety of typologies or paradigms. Detailed descriptions on the use of ANNs in environmental modelling can be found in Maier and Dandy (2000) [22].

III.MODEL DEVELOPMENT

In order to identify the changes in regional levels of CO concentration annual average values of mid day (06.00 – 14.00 hrs) 8 hourly average carbon monoxide concentration data is plotted as in Figure (2). It is obvious from the graph that there is sudden rise in ambient CO levels after the year 1999 till the year 2001 owing to the rise in polluting vehicle numbers. After the year 2000 with the enforcement of several pollution control norms there has been a marked decrease in the CO levels but not to the satisfactory level since concentration was not below the norms 2000 µg/m^3.

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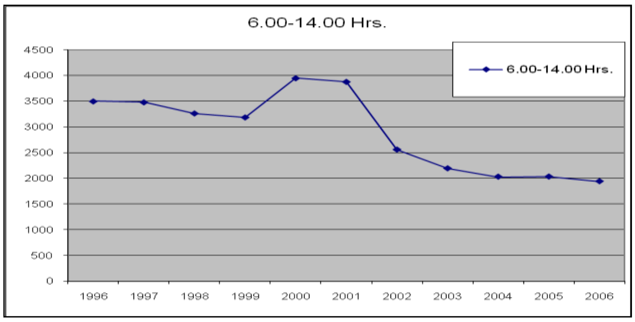

Figure (2) - Trends in Yearly Average CO Concentration.

Based upon the analysis of CO trend the analysis of data is classified into three groups (stages) as listed in the Table II below. Accordingly, between the years 1996-2000 (the pre intervention period) the air pollution control regulations have been forced to be adopted by all the concerned. With the time the stringent enforcement of pollution control measures have resulted in improved air quality after the year 2003.

Table II- Classification of CO data for ANN Analysis

Group	Duration	Data Length	Reason for Classification
A	Jan. 1996 – Dec.1999	4 years	Pre Intervention Period
B	Jan. 2000 – Dec. 2002	3 years	Transition Phase
C	Jan. 2003 – Dec. 2005	3 years	Post Implementation duration
D	Year 2006 data is exclusively used for model forecast purposes		

In the Figure (3) annual CO values are represented by their mean, median, mode, standard deviation (S.D.) and sample mean (SM+ and SM-) with 95% confidence level. The larger values of sample mean in comparison to the mode and median values is indicative of larger dispersion of data which is further supported by the higher standard deviation in the data. The higher mode value during the year 2002 is the indication of the exceptionally large frequency of few higher CO concentrations.

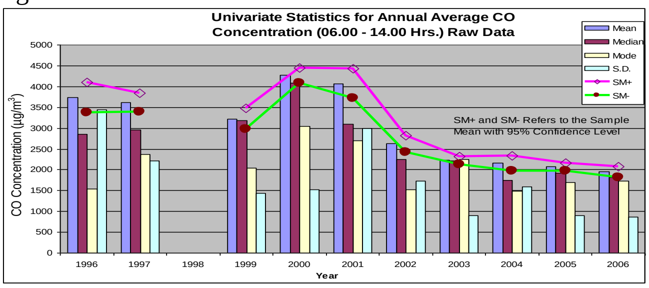

Figure (3)-Elementary Statistics of Av. (8 Hr) CO data

For ANN modelling the available data is divided into three set: training / learning set, validating set and testing set. These sets can overlap and do not have to be continuous. The complete process of ANN prediction used in this study can be summed as –

- The Train / Test data set Selection from the given time series for model building is done in such a way that the test set is statistically close to the training set and hold back a portion of data for independent model validation.
- Next the Input Variable Selection is done using a genetic algorithm. Advantage is that the different initializations of the algorithm yield different variable sets and thus we have several models based on different variable sets and combine the outputs of those models. Each model can be thought of as an expert which uses a different set of criteria to make its decision.
- The number of hidden layer neurons was determined using the trial and error procedure for each model under each of the data category described earlier.
- For building MLP models the general purpose algorithm based on an Adaptive Gradient learning rule has been used. Multiple networks are trained for optimal results and many different evaluation functions are estimated for evaluating test performance during training.
- The unipolar sigmoid activation function and the generalized delta rule were employed in all the ANN models developed in this study. Once the best ANN architectures for each data category were obtained, they were used to compute the performance statistics during both training and testing.

Table III, gives details of ANN design (learning) parameters and selected architectures, for forecasting of mid day (06.00 – 22.00 Hrs) 8 hourly CO observations at the same time, one day and two day advance (Lag 0, 1 and 2) periods. In the Table-III abbreviations are as NNA = Neural Network Architecture, I:H:O = Input:Hidden:Output layer Architecture, R is the correlation coefficient with its absolute value as net R. Absolute maximum and average absolute values of forecasted data are given with root mean square (RMS), forecast efficiency and 95% confidence level (CL).

Table-III ANN Design Parameters for CO Concentration (06.00-14.00 Hrs.)

SN	Input	Output	I:H:O	Time Lag	Data Set	R	Net R	Max. Abs.	RMS	Accuracy	95% CL	Record
1	Jan. – Mar., & Oct. – Dec.; 1996 -1998	Jan. – Mar., Oct., -Dec., 1999	1:7:2	L=0	All	1	-1	794	176	1	342	495
					Train	1	-1	794	175	1	342	346
					Test	1	-1	794	176	1	346	149
					Valid	1	-1	794	176	1	342	495
			1:2:2	L=1	All	0.6	-0.6	6697	1775	0.8	3461	495
					Train	0.5	-0.5	6697	1797	0.8	3507	346
					Test	0.6	-0.6	6309	1725	0.8	3553	149
					Valid	0.6	-0.6	6697	1775	0.8	3598	495
			1:4:3	L=2	All	0.3	-0.3	7123	2014	0.8	3926	495
					Train	0.3	-0.3	7123	2001	0.7	3905	346
					Test	0.3	-0.3	6851	2044	0.8	4012	149
					Valid	0.3	-0.3	7123	2014	0.8	3926	495
2	Jan.- Mar., & Oct. Dec.; 2000 -2001	Jan. – Mar., Oct., -Dec., 2002	1:4:3	L=0	All	1	-1	623	139	1	271	365
					Train	1	-1	623	140	1	274	255
					Test	1	-1	623	136	1	267	110
					Valid	1	-1	623	139	1	271	365
			1:6:3	L=1	All	0.7	-0.7	6335	1437	0.8	2804	365
					Train	0.7	-0.7	4135	1433	0.8	2802	255
					Test	0.8	-0.8	6335	1446	0.9	2848	110
					Valid	0.7	-0.7	6335	1437	0.8	2804	365
			1:0:3	L=2	All	0.6	-0.6	6419	1679	0.8	3276	365
					Train	0.6	-0.6	6419	1702	0.8	3327	255
					Test	0.6	-0.6	5867	1624	0.8	3199	110
					Valid	0.6	-0.6	6419	1679	0.8	3276	365
3	Jan. –	Jan. –	1:2:3	L=0	All	1	-1	735	140	1	273	512

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	Mar., & Oct. - Dec.; 2003-2005	Oct., 2006			Train	1	-1	735	140	1	273	358
					Test	1	-1	735	139	1	274	154
					Valid	1	-1	735	140	1	273	512
			1:0:2	L=1	All	0.5	-0.5	6001	1739	0.7	3390	512
					Train	0.5	-0.5	6001	1732	0.7	3381	358
					Test	0.5	-0.5	5162	1755	0.7	3443	154
					Valid	0.5	-0.5	6001	1739	0.7	3390	512
			1:1:2	L=2	All	0.3	-0.3	5998	1851	0.6	3608	512
					Train	0.4	-0.3	5998	1846	0.7	3602	358
					Test	0.4	-0.3	5588	1863	0.6	3657	154
					Valid	0.3	-0.3	5998	1851	0.6	3608	512

The forecasts are made for the months of Oct. to Mar.(year 1999 and 2002) and Jan. to Oct. (year 2006) and graphically presented in figure (4). Forecasting is done for the winter months since the weather remains moderately stable for CO spread. During summer and monsoon months respective highly unstable and wash out conditions inherit better forecasts. For most of the time the forecasted values are in tune with the observed CO conc. in trends and pattern. It is found that the NN perform absolutely well for lag zero (L=0) forecasting with around 99% accuracy followed by the one day (L=1) and two days (L=2) ahead forecasts with 70-80% and 50-80% accuracy respectively.

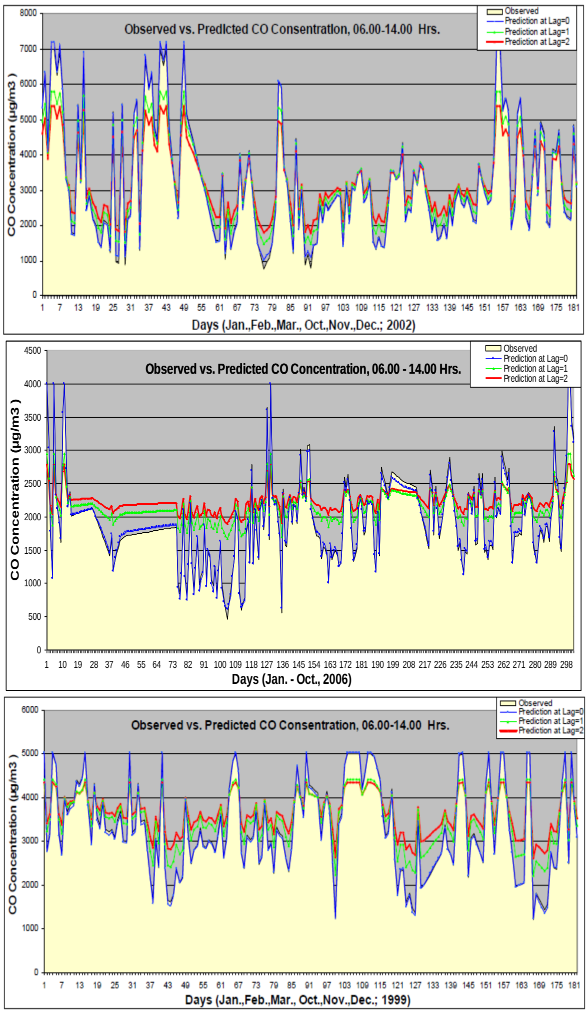

Figure (4)- Univariate CO Time Series Forecast Using Neural Network for the years (1999, 2002, and 2006)

IV. MODEL TESTING AND VALIDATION

The performance of all the models has been evaluated using the statistical parameters and tabularize in Table (4) as recommended by willmott & Masuura (2005) [23] and

Table (4)- Statistical Evaluation of CO Forecast

SN	Duration	Lag	Std. Dev.		Errors				RMSE	CD	IA	FB	FAC2
			O	P	MPE	MBE	MAE	NMSE	T				
1	Jan., 1999	L=0	711	729	0	-44.3	51.9	0	56.9	1	1	0	1
		L=1	711	368	0	46.4	295.7	0	343.1	1	0.9	0	1
		L=2	711	294	0	96.6	366.7	0	422.4	1	0.8	0	1
2	Dec., 1999	L=0	1306	1320	0	-18	38.3	0	47.2	1	1	0	1
		L=1	1306	770	0	231.9	525.2	0	581.3	1	0.9	-0.1	1
		L=2	1306	588	0	394.6	718.7	0.1	810.8	1	0.8	-0.1	1
3	Jan., 2002	L=0	2113	2141	0	33.5	76.2	0	104.4	1	1	0	1
		L=1	2113	1550	0	-92.8	466.2	0	573.9	1	1	0	1
		L=2	2113	1257	0	-108	732.3	0	852.8	1	0.9	0	1
4	Dec., 2002	L=0	1499	1531	0	-23.6	50.2	0	68.2	1	1	0	1
		L=1	1499	1136	0	-107	284.4	0	393.5	1	1	0	1
		L=2	1499	903	0	-184	503.7	0	618.8	1	0.9	0	1
5	Jan., 2006	L=0	706	695	0	-7.7	23.7	0	35.8	1	1	0	1
		L=1	706	275	0	-33.6	292.2	0	425.7	1	0.8	0	1
		L=2	706	190	0	15.3	376.2	0	507.8	1	0.7	0	1
6	Oct., 2006	L=0	730	696	0	-6.1	45.3	0	52	1	1	0	1
		L=1	730	278	0	12.5	353.6	0	445.6	1	0.8	0	1
		L=2	730	193	0	68.6	431.5	0.1	532.7	1	0.7	0	1

Schlink et. al (2006) [24]. The performance of Neural network models are evaluated for the January and December months of the year 1999 and 2002 and for the months of January and October for the year 2006 . To provide a numerical description of the goodness of the estimates we have used some selected statistical parameters viz. –

1. Standard deviations of observed (O) and predicted data(P) = $\sqrt{\frac{1}{N-1}\sum(O_i-\overline{O})^2}$

2. Mean Percentage Error (MPE)

$$= \frac{1}{N}\left(\sum_{i=1}^{N} PE_i\right)$$

3. Mean Biased Error (MBE)

$$= \frac{\sum_{i=1}^{n} e_i}{n} = \frac{\sum_{i=1}^{n}(P_i - O_i)}{n} = \overline{P} - \overline{O}$$

4. Mean Absolute Error (MAE),

$$= \frac{1}{N}\sum\left|O_i - \overline{O}\right|$$

5. Normalised mean square error (NMSE)

$$= \frac{\overline{(O-P)^2}}{\overline{O}\,\overline{P}}$$

6. Root mean square error (RMSE) is the most common indicators used with neural networks is calculated as-

$$= \sqrt{\frac{\sum_{i=1}^{n}\left|(P_i - O_i)\right|^2}{n}}$$

7. The Coefficient of Determination (CD) / Pearson's R **squared** (R^2),:-

$$R^2 = \left[\frac{\sum_{i=1}^{n}(O_i-\overline{O})(P_i-\overline{P})}{\sqrt{\sum_{i=1}^{n}(O_i-\overline{O})^2\sum_{i=1}^{n}(P_i-\overline{P})^2}}\right]^2$$

8. Fractional Bias (FB)

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$$FB = \frac{2(\bar{O} - \bar{P})}{(\bar{O} + \bar{P})} \qquad where \quad \bar{O} = \frac{\sum_{i=1}^{n} O_i}{n} \; and \; \bar{P} = \frac{\sum_{i=1}^{n} P_i}{n}$$

9. Factor within 2 (FAC2) are also evaluated

10. Index of agreement (IA):- The IA is a descriptive statistics that reflects the degree to which the observed variate is accurately estimated by the simulated model. The index of agreement is not a measure of correlation or association in the formal sense, but rather a measure of the degree to which model predictions are error free and it is a standardized measure. It varies between 0 and 1. A computed value of 1 indicates perfect agreement between the observed and predicted observations, while 0 connotes complete disagreement (Willmott 1981) [25]. The value of IA =

$$1 - \frac{\sum_{i=1}^{n}(P_i^{'} - O_i^{'})^2}{\sum_{i=1}^{n}\left(\left|P_i - \bar{O}\right| + \left|O_i - \bar{O}\right|\right)^2} = 1 - \frac{\sum_{i=1}^{n}(P_i - O_i)^2}{\sum_{i=1}^{n}\left(\left|P_i - \bar{O}\right| + \left|O_i - \bar{O}\right|\right)^2}$$

where, N is number of the data points; O_i observation data points; P_i predicted data points; $\bar{O}$ mean of the observed data points

V.CONCLUSION

The prepared NN forecasts are for the lag zero, one and two hour duration. It is clear from the Figure (4) that the forecasts at lag 0 are outstandingly best and are close to observed CO levels. The forecasting performance of model reduces with the increasing time lag. The standard deviations of morning time CO forecasts using univariate NN modelling shows a gradually decreasing trend as the time lag increases. The MPE are nearly zero indicating a close proximity between observed and forecasted values of CO using NN. MBE, MAE, and RMSE are according to their relative arrangement (distribution of data). NMSE and fractional bias are close to the zero indicating very good agreement of forecasted values with the observed one.

The coefficient of determination for this case is nearly 1.0 indicating high correlation between the patterns of forecasts and observed values, however, IA values limits the fact by representative the percentage of association in the range of 100 to 90 % for lag 0, 100 to 80% for lag 1 and 90 to 70% for lag 2 forecasts. The best forecasts are for the month of January since the weather remains mostly calm and stable due to acute winter season. Overall performance of the forecasts is on the top for the year 2002 followed by the forecasts of the year 1999 and 2006.

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