Nature Environment and Pollution Technology
An International Quarterly Scientific Journal
p-ISSN: 0972-6268 (Print copies up to 2016)
e-ISSN: 2395-3454
Vol. 23 | No. 1 | pp. 525-535 | 2024
Original Research Paper
https://doi.org/10.46488/NEPT.2024.v23i01.049
Open Access Journal

A Short-Term Autoregressive Model for the Prediction of Daily Average NO_2 Concentration in Nagercoil, Tamil Nadu, India

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Nat. Env. & Poll. Tech.
Website: www.neptjournal.com

Received: 04-07-2023
Revised: 12-08-2023
Accepted: 21-08-2023

Key Words:
Akaike information criterion
Autoregressive model
Diurnal changes
Jarque-Bera test
NO_2

ABSTRACT

Nitrogen dioxide (NO_2) is one of the pollutants that can cause potential damage to the ecosystem. NO_2 emitted from vehicles forms the primary precursor for ground-level ozone. In this study, an analysis of the daily average of NO_2 concentration with meteorology measured for two years 2021 and 2022 is being carried out. It is evident from the analysis that NO_2 concentration followed an apparent diurnal pattern with a maximum value in the morning hours and a minimum during the afternoon hours. Summer months recorded the highest, and North East Monsoon (NEM) recorded the lowest values of NO_2. A statistically significant positive correlation was found between NO_2 and Temperature. An autoregressive model was formulated to forecast the daily average values of NO_2 concentration. Unit root test was performed to check the stationarity of the data points, which is important in determining trends and seasonal changes. From the model procedure, the order that best fits the data was identified as AR (4), in which the process has the current value based on the previous three values. The Akaike Information Criterion (AIC) and Schwartz Criterion (SC), which are estimators of prediction error for AR (4), are low. The Jarque confirmed the normal distribution-Bera test, which again approves the satisfactoriness of the model..

INTRODUCTION

Nitrogen Dioxide (NO_2) is a prominent potential pollutant and is formed in the atmosphere through the oxidation of nitric oxide (NO). NOx is the broader term that comprises the other oxides of nitrogen. NO_2 is a very reactive and significant species in the atmosphere, and vehicle transport plays a major role in increasing NO_2 concentrations (Lawrence et al. 2015). It plays a significant part in the formation of tropospheric ozone, as an aerosol-producing agent, and in the production of acidic species (Logan 1983, Pitts & Pitts 1986). Nitrogen dioxide (NO_2) is mainly affected by local emissions and meteorology rather than long-range transport (Yin et al. 2022). Ambient sources of NOx can be categorized into anthropogenic and natural sources, but the major contribution is from anthropogenic sources. It is to be noted that the majority of the countries consider NO2 concentration as an important indicator of air quality (Xue et al. 2020). Estimates of lightning-based NOx emissions for North America range from 1.2 to 1.7 $Tg.y^{-1}$ of NO_2 (Placet et al. 1990). Crutzen & Schmailz (1983) estimated global NOx emissions from stratospheric injection to be 0.5 $Tg.y^{-1}$. Numerous studies are showing a steady relationship between NO_2 exposure with reduced lung activity and increased respiratory symptoms (Ackermann-Liebrich 1997, Schindler 1998, Smith 2000). NO_2 causes bronchiolitis obliterans, a serious condition within a couple of weeks after exposure to around 150 ppm. NO_2 exposure of 500 ppm causes terminal illness (Gauderman et al. 2000). Chiusolo et al. (2011) found that there is a strong relationship between the rise in NO_2 and the mortality rate. Gurjar et al. (2010) estimated that elevated levels of NO_2 and SO_2 resulted in more number of deaths in Mumbai and Delhi. There exists a high correlation between NO_2 concentration and other pollutants that are formed through some chemical reactions (Burnett et al. 2007). NO_2 is an efficient absorber of visible radiation, and it has been projected as a plausible source of additional climatic influences (Wuebbles et al. 1989). Several mathematical models have been developed for forecasting pollutants in the atmosphere. The effects of elevated levels of NOx in China were investigated by Liu et al. (2003) using a three-dimensional chemical model. Multilayer Perceptron models were used in the prediction of NOx and NO_2 levels (Gardner & Dorling 1998). Lengyel et al. (2004) proposed a principal component analysis for analyzing NO_2. Many air-quality studies use PCA to develop statistically independent basic components (Maenhaut et al. 1989). Statheropoulos et al. (1998) and Vaidya et al. (2000) examined the pollutant concentration with the use of component analysis. Recently, predictions for Fuzzy time series were performed using a multivariate heuristic model (Huarang et al. 2007), and a new method using Fuzzy relation based on a neural network algorithm was suggested for high-dimensional time series data (Egrioglu et al. 2009). These models must gratify many conditions and constraints (Isufi et al. 2019). This work aims to examine the variation of nitrogen dioxide concentration and forecast the daily average concentration of NO_2 for a short term using Autoregressive Integrated Moving Average (ARIMA) time series model.

MATERIALS AND METHODS

Study Area and Data Collection

Nagercoil (8.1833 N 77.4119 E) is one of the busy traffic-prone towns of south Tamil Nadu. Also, there are many brick kiln industries in and around that emit NOx into the atmosphere. To analyze the lifetimes, accumulation, and impacts, it is vital to know the interactions among various trace gases in the atmosphere. Studies suggest that NO_2 in traffic or on throughways can be two times as high as levels observed in residential areas. Fig.1 shows the study area and NO_2 monitor.

There are various mathematical models available for predicting the pollutants. Generally autoregressive (AR) model is a representation to study some time-varying processes in the environment. In particular, an ARIMA model was formulated for predicting the daily average values of NO_2 concentration.

Analysis

To carry out the optimization of various variables, including the number of parameters, criteria like Akaike's Information Criteria (AIC) and Bayesian Information Criteria (BIC), accuracy, and easiness of implementation, an autoregressive model was chosen. The estimation of the coefficients was carried out using "Eviews" software. In time series analysis, Auto Regressive Moving Average (ARMA) or Auto-Regressive Integrated Moving Average (ARIMA) models are generally proposed for better futuristic prediction (Adejumo & Momo 2013, Chattha 2021). This approach essentially has the following stages.

Stationarity test: In ARIMA modeling, it is noted that the data has to be changed to stationary form before doing analysis. It is easy to model when the data on a time series is stationary. Statistical modeling requires the data to be stationary for the effective forecast. If the data

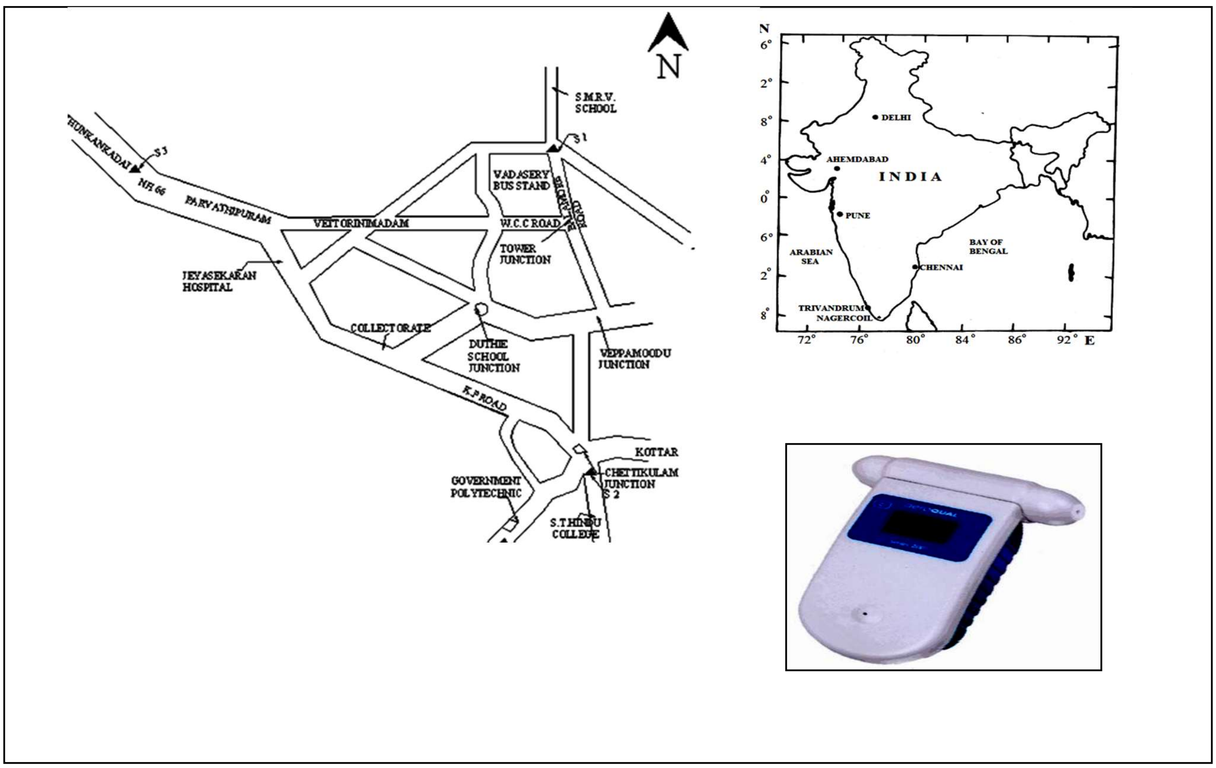


Fig. 1: Study area and monitor.

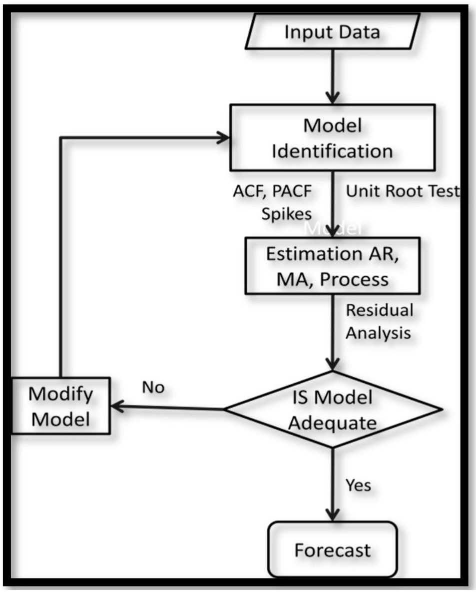


Fig. 2: Steps to be followed in modeling.

shows some trend, removal of the trend is vital. First, differencing is suitable for detrending the data points. Unit root tests (Dickey-Fuller tests) help to decide whether data should be first differenced or regressed. A stationary time series is significant in forecasting if the series is non-stationary.

Consider a time series equation, Z (t), such that

$$\{Z (t), t=1,\ldots\ldots \infty\}.$$

Suppose the AR term of p^{th} order is written as

$$Z_t = a_1 y_{t-1} + a_2 y_{t-2} + \ldots\ldots apyt_{-p} + £_t \qquad \ldots(1)$$

The error term $£_t$ should have constant variance and must not be serially uncorrelated. If any one of the roots of equation (1) is equal to unity, then it has a unit root. This shows the non-stationarity of the series. The successive differencing methods reduce the trend effects and give the stationary series.

Autocorrelation plots: The autocorrelation function (ACF) and partial autocorrelation function (PACF) plots are useful for determining the number of values that are statistically significant over the different lagged periods. The significant spikes of PACF are used for determining the order of the autoregressive model and vice versa. The parameters of the ARMA model are characterized by the orders of both auto-regressive and moving average series. The primary step is to determine the suitable models using the functions ACF and PACF (Sharma et al. 2009). The process of identification is the most vital and also the most challenging step (Dobre & Alexandru 2008).

Diagnostic Check and Forecast

Diagnostic Check has turned out to be a regular tool for the identification of models before predicting the data. This check is applied to assess the residuals from the model when a model is estimated and also serves as the test of model adequacy. In specific, the residuals must not be dependent on one another and should be invariant in mean and deviation (Adejumo & Momo 2013). Suppose the residuals are not correlated, and the histogram follows a Gaussian distribution with mean zero and constant variance. In that case, the model is considered to be correct, and the data can be forecasted. In this work, we have used various kinds of software like Microsoft Excel (MS Excel) and Eviews 7 for creating the ARIMA model. Fig. 2 shows the various steps involved in modeling.

RESULTS AND DISCUSSION

Diurnal Variation

The distribution of the daily average of NO_2 and meteorological parameters is depicted in Fig. 3. The overall averaged diurnal variation is represented in Fig. 4. The minimum value of averaged diurnal NO_2 concentration was found to be 1.86 ppb, and the maximum value was 6.49 ppb. The diurnal cycle showed two characteristic peaks in a day. The appearance of the first peak was at 08:30 H, and the next peak was around 23:30 H. The maximum value was recorded during nighttime. The gradual increase in NO_2 concentration from early morning to 0830 H was mainly due to the increase in vehicular flow. This is also related to the features of nighttime boundary layer height (Teixeira et al. 2009). A minimum value was noticed at noon time, around 1430 H. Since NO_2 gets converted to ozone in the presence of sunlight, the drop in NO_2 was mainly due to this conversion in the selected site. The photochemical reaction stops after sunset, and hence, the conversion rate decreases, resulting in the build-up of NO_2 concentration.

Variation of NO_2 with Meteorology

The overall variation of daily average NO_2 concentration for two years is given in Fig. 5. The daily average recorded a minimum of 3.16 ppb and a maximum of 6.88 ppb. The matrix plot of NO_2 and meteorological parameters such as temperature, RH, and wind speed is depicted in Fig. 6. The analysis showed a positive correlation of 0.473 ($p<0.05$) between NO_2 and temperature, whereas for NO_2 and RH was significantly negative with a coefficient of -0.237. A weak correlation between NO_2 and wind speed was noted with a coefficient value of 0.192.

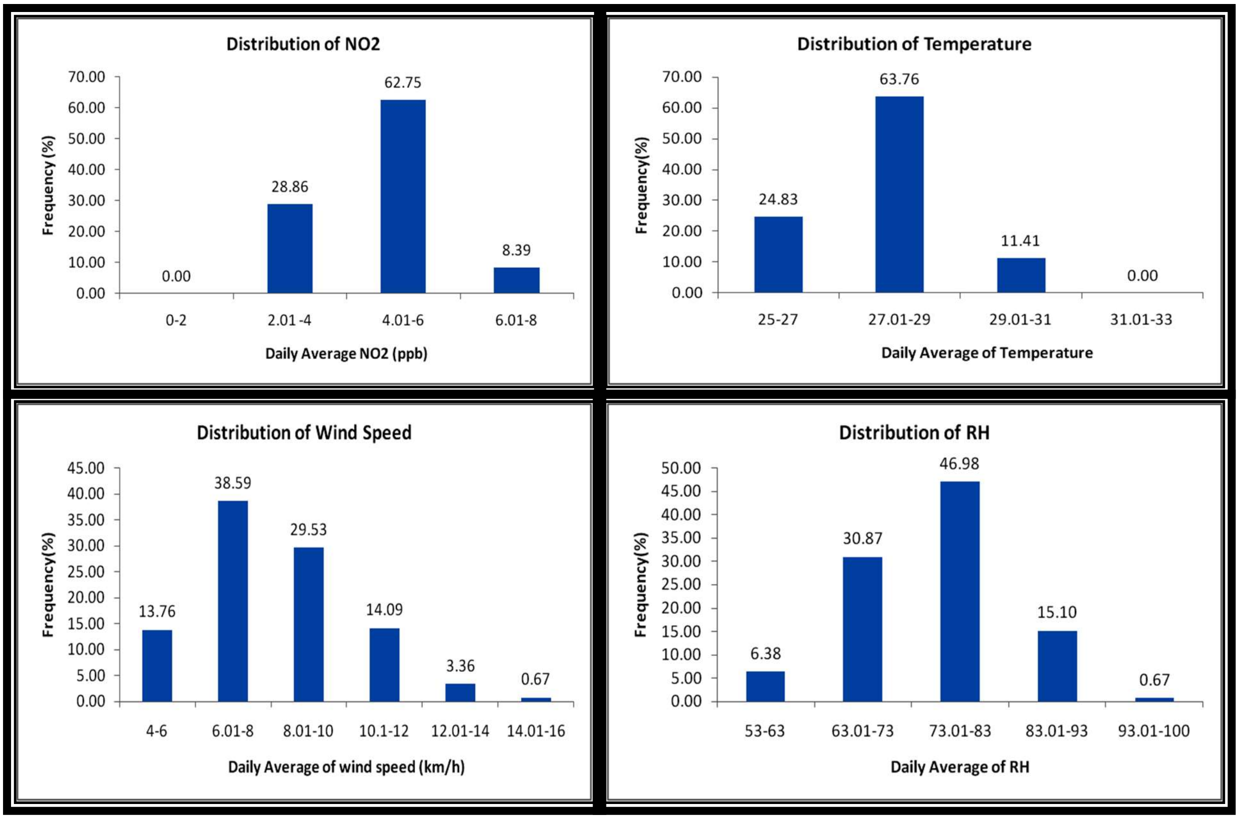


Fig. 3: Frequency distribution.

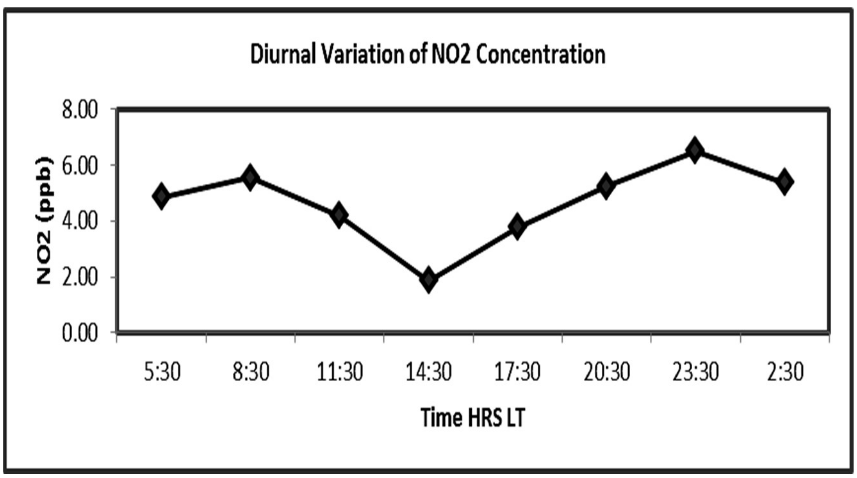


Fig. 4: Diurnal variation of NO_2.

Seasonal Variation

The seasonal division of Nagercoil City is in accordance with the meteorological standard of the Indian Meteorological Department (IMD). Summer is from March to May, and South West Monsoon (SWM) extends from June to September. North East Monsoon (NEM) starts in October and ends in December. January and February are winter months. The seasonal variation of NO_2 and meteorological parameters is depicted in Fig. 7. For both years, the summer season recorded the highest daily average concentration of NO_2, followed by SWM. This may be because of the high oxidation rate of Nitric oxide (NO) to NO_2 and also due to conversion by ozone. Lowest values of NO_2 were recorded in NEM for both years owing to the pollutant washout due to monsoon rain. There is an increase in the daily average NO_2 concentration moving from NEM to winter. The high values of NO_2 in winter are attributed to relatively low temperatures and the accumulation of the pollutant. This is inconsistent with the study reported by Wang et al. (2019).

ARIMA (Box-Jenkinson) Model

Box-Jenkins Analysis discusses an orderly way of recognizing, fitting, and testing, uses moving average time series models, and is suitable for time series of moderate intervals. This work mainly aims to forecast daily averaged nitrogen dioxide concentration. The first step is to trace out the presence of seasonality in the data set and to

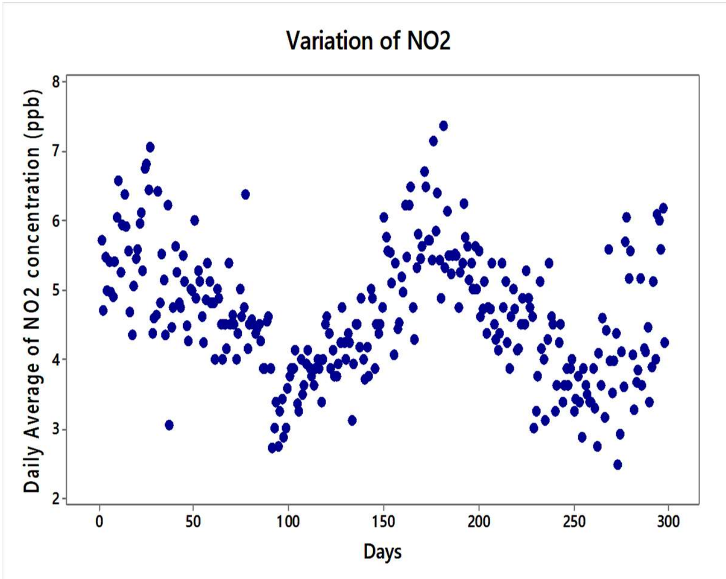


Fig. 5: Overall variation of NO_2.

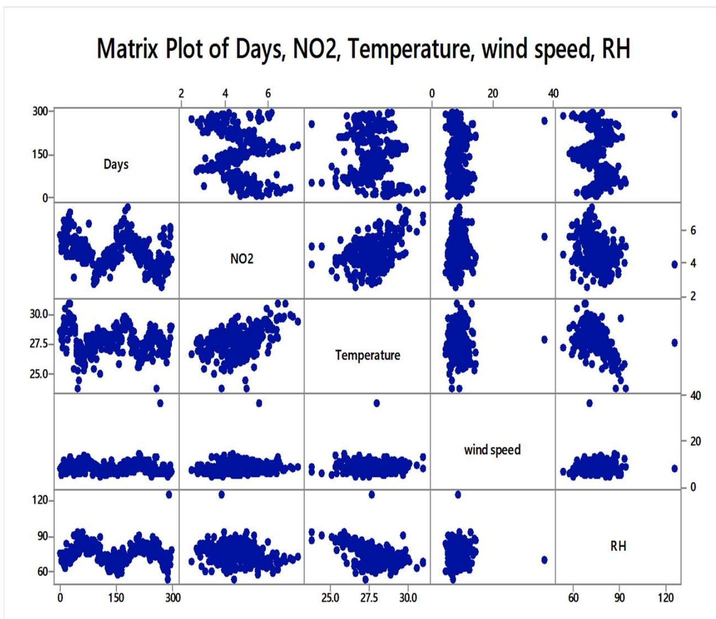


Fig. 6: Matrix plot of NO_2 and meteorology.

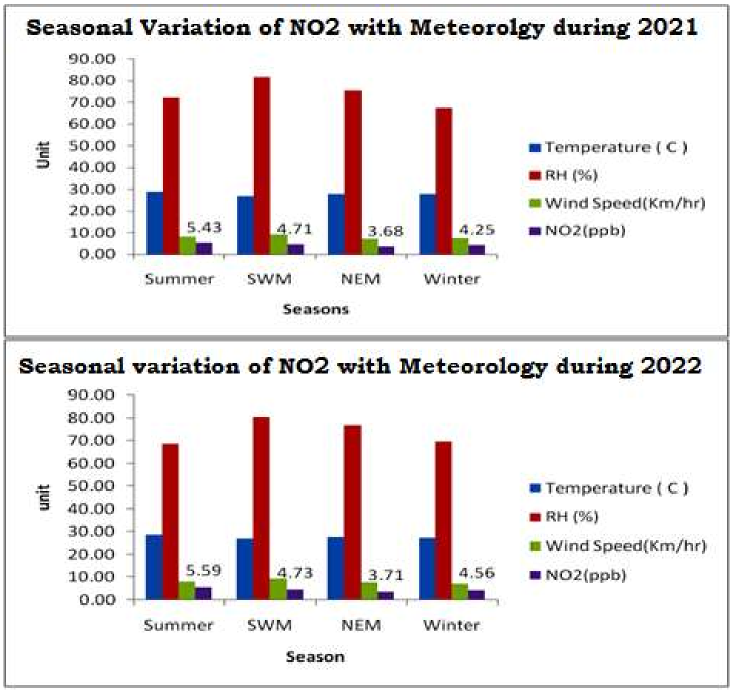


Fig. 7: Seasonal variation of NO_2.

deseasonalize the data. Unit root analysis was performed with the Augmented Dickey-Fuller test for 40 lags to elucidate the seasonality. Fig. 8 depicts the raw data with seasonal patterns. The data points were deseasonalized after performing the first difference, and the probability value became zero, which is given in Fig. 9. The test results display that statistics Dickey-Fuller (-10.86681) is smaller than the threshold values (-3.500669, 2.892200, and -2.583192) relating to critical thresholds of one percent, five percent, and ten percent, respectively. Thus, it is concluded that the series does not have a unit root and is stationary. The correlogram of the data series after removing seasonality is given in Fig. 10.

The next step is to identify the relevant ARMA (p, q) process. This is done by examining the ACF and PACF of the data for selecting the most favorable autoregressive and moving average terms of the model to be selected. From the plot, it can be noted that the simple function of autocorrelation exhibits a minor peak at shift 1, whereas the partial autocorrelation function has peaks up to shift 4. Therefore, it is reasonable to suspect that a moving average of the first order and autoregressive term of the fourth order would be a suitable estimate. Thus, the models AR (1), MA (1), AR (1 2 3 4), and ARMA (4 1) are identified. The performance of the identified models was verified based on

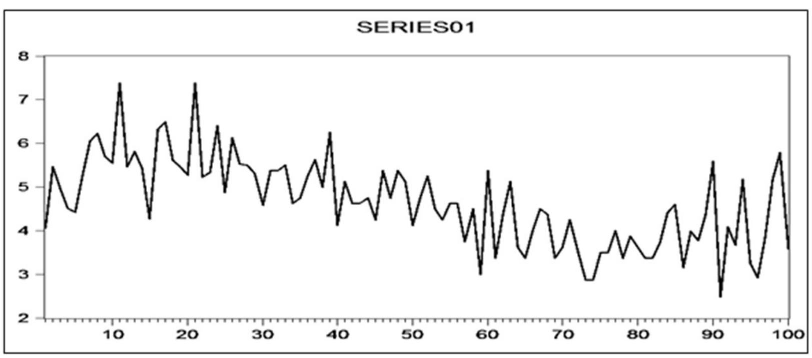


Fig. 8: Raw data with seasonality.

Null Hypothesis: D(SERIES01) has a unit root
Exogenous: Constant
Lag Length: 3 (Automatic - based on SIC, maxlag=40)

		t-Statistic	Prob.*
Augmented Dickey-Fuller test statistic		-10.86681	0.0000
Test critical values:	1% level	-3.500669	
	5% level	-2.892200	
	10% level	-2.583192	

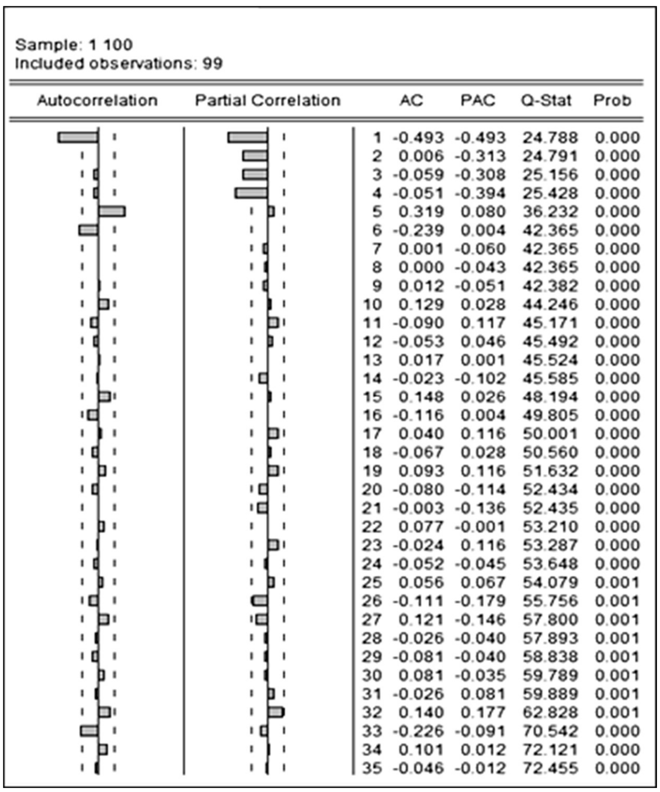
*MacKinnon (1996) one-sided p-values.

Augmented Dickey-Fuller Test Equation
Dependent Variable: D(SERIES01,2)
Method: Least Squares
Date: 11/09/16 Time: 17:01
Sample (adjusted): 6 100
Included observations: 95 after adjustments

Variable	Coefficient	Std. Error	t-Statistic	Prob.
D(SERIES01(-1))	-3.874626	0.356556	-10.86681	0.0000
D(SERIES01(-1),2)	1.946170	0.296759	6.558090	0.0000
D(SERIES01(-2),2)	1.137050	0.205217	5.540727	0.0000
D(SERIES01(-3),2)	0.444364	0.100436	4.424326	0.0000
C	-0.011767	0.074141	-0.158716	0.8742

R-squared	0.837246	Mean dependent var	-0.022247
Adjusted R-squared	0.830012	S.D. dependent var	1.751567
S.E. of regression	0.722163	Akaike info criterion	2.238064
Sum squared resid	46.93675	Schwarz criterion	2.372479
Log likelihood	-101.3080	Hannan-Quinn criter.	2.292378
F-statistic	115.7454	Durbin-Watson stat	1.920820
Prob(F-statistic)	0.000000		

Fig. 9: Output of unit root test after removing seasonality.


Sample: 1 100
Included observations: 99

Autocorrelation	Partial Correlation		AC	PAC	Q-Stat	Prob
		1	-0.493	-0.493	24.788	0.000
		2	0.006	-0.313	24.791	0.000
		3	-0.059	-0.308	25.156	0.000
		4	-0.051	-0.394	25.428	0.000
		5	0.319	0.080	36.232	0.000
		6	-0.239	0.004	42.365	0.000
		7	0.001	-0.060	42.365	0.000
		8	0.000	-0.043	42.365	0.000
		9	0.012	-0.051	42.382	0.000
		10	0.129	0.028	44.246	0.000
		11	-0.090	0.117	45.171	0.000
		12	-0.053	0.046	45.492	0.000
		13	0.017	0.001	45.524	0.000
		14	-0.023	-0.102	45.585	0.000
		15	0.148	0.026	48.194	0.000
		16	-0.116	0.004	49.805	0.000
		17	0.040	0.116	50.001	0.000
		18	-0.067	0.028	50.560	0.000
		19	0.093	0.116	51.632	0.000
		20	-0.080	-0.114	52.434	0.000
		21	-0.003	-0.136	52.435	0.000
		22	0.077	-0.001	53.210	0.000
		23	-0.024	0.116	53.287	0.000
		24	-0.052	-0.045	53.648	0.000
		25	0.056	0.067	54.079	0.001
		26	-0.111	-0.179	55.756	0.001
		27	0.121	-0.146	57.800	0.001
		28	-0.026	-0.040	57.893	0.001
		29	-0.081	-0.040	58.838	0.001
		30	0.081	-0.035	59.789	0.001
		31	-0.026	0.081	59.889	0.001
		32	0.140	0.177	62.828	0.001
		33	-0.226	-0.091	70.542	0.000
		34	0.101	0.012	72.121	0.000
		35	-0.046	-0.012	72.455	0.000

Fig. 10: Correlogram of the data after removing seasonality.

Dependent Variable: D(SERIES01)
Method: Least Squares
Date: 11/09/16 Time: 17:06
Sample (adjusted): 6 100
Included observations: 95 after adjustments
Convergence achieved after 3 iterations

Variable	Coefficient	Std. Error	t-Statistic	Prob.
C	-0.003037	0.019131	-0.158750	0.8742
AR(1)	-0.928456	0.095856	-9.685952	0.0000
AR(2)	-0.809120	0.120348	-6.723156	0.0000
AR(3)	-0.692686	0.124394	-5.568474	0.0000
AR(4)	-0.444364	0.100436	-4.424326	0.0000

R-squared	0.519611	Mean dependent var	-0.008821
Adjusted R-squared	0.498261	S.D. dependent var	1.019521
S.E. of regression	0.722163	Akaike info criterion	2.238064
Sum squared resid	46.93675	Schwarz criterion	2.372479
Log likelihood	-101.3080	Hannan-Quinn criter.	2.292378
F-statistic	24.33707	Durbin-Watson stat	1.920820
Prob(F-statistic)	0.000000		

Inverted AR Roots	.20+.82i	.20-.82i	-.66-.43i	-.66+.43i

Fig. 11: Output of the estimated model.

Akaike Information Criterion (AIC), Schwartz Criterion (SC), Histogram Normality test, and residuals check. The output obtained after estimating the equation for the AR (4) model is given in Fig. 11. From the table, it is evident that the probability values tend to be zero, and the AIC and SC values are getting lowered. In statistics, the Schwarz criterion is a condition for model selection among a limited set of models. The model with the least BIC is preferred.

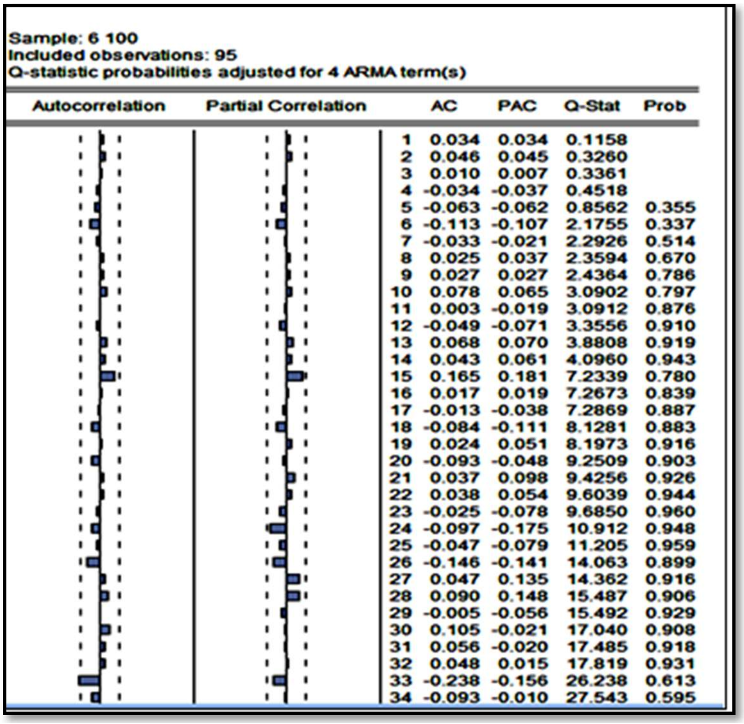
Two criteria normally used are the Akaike Information Criterion (AIC) and the Schwarz Criterion (SC; also known as the Bayesian information criterion or BIC).

Table 1 gives the estimated output of the various identified models. From the table, it is confirmed that the model AR (1 2 3 4) has the least value for AIC and SC. The right model can be chosen for that which reduces the Akaike Information Criterion (AIC) and the Schwarz Criterion (SC) values. To confirm the adequacy of the selected model, it is important to test residuals. The analysis involves checking whether the residuals are inside the upper limit. Hence, the sample ACF and PACF of the residuals were tested to check whether they do not follow any pattern and are strongly significant. The correlogram of the residuals is shown in the Fig. 12.

The histogram–normality distribution of the selected model is given in Fig. 13. The Jarque-Bera test allows us to assess the residual normality. The null hypothesis is that the residuals follow the Gaussian distribution. From Fig. 13, the normal distribution of the data is evident. If the Jarque-Bera value is higher than the chi-square critical value with two degrees of freedom, the alternate hypothesis must be accepted. The Jarque-Bera test statistic of 1.219970 is less than the chi-square critical value of 5.99 at the five

Table 1: Comparison of AIC & SC for identified models.

Identified models	AIC	SC	P-value
AR(1)	2.6360	2.659	0.000
MA(1)	2.3302	2.3535	0.000
ARMA(4 1)	2.2768	2.4200	0.889
AR(4)	2.2380	2.3724	0.000


Sample: 6 100
Included observations: 95
Q-statistic probabilities adjusted for 4 ARMA term(s)

Autocorrelation	Partial Correlation		AC	PAC	Q-Stat	Prob
		1	0.034	0.034	0.1158	
		2	0.046	0.045	0.3260	
		3	0.010	0.007	0.3361	
		4	-0.034	-0.037	0.4518	
		5	-0.063	-0.062	0.8562	0.355
		6	-0.113	-0.107	2.1755	0.337
		7	-0.033	-0.021	2.2926	0.514
		8	0.025	0.037	2.3594	0.670
		9	0.027	0.027	2.4364	0.786
		10	0.078	0.065	3.0902	0.797
		11	0.003	-0.019	3.0912	0.876
		12	-0.049	-0.071	3.3556	0.910
		13	0.068	0.070	3.8808	0.919
		14	0.043	0.061	4.0960	0.943
		15	0.165	0.181	7.2339	0.780
		16	0.017	0.019	7.2673	0.839
		17	-0.013	-0.038	7.2869	0.887
		18	-0.084	-0.111	8.1281	0.883
		19	0.024	0.051	8.1973	0.916
		20	-0.093	-0.048	9.2509	0.903
		21	0.037	0.098	9.4256	0.926
		22	0.038	0.054	9.6039	0.944
		23	-0.025	-0.078	9.6850	0.960
		24	-0.097	-0.175	10.912	0.948
		25	-0.047	-0.079	11.205	0.959
		26	-0.146	-0.141	14.063	0.899
		27	0.047	0.135	14.362	0.916
		28	0.090	0.148	15.487	0.906
		29	-0.005	-0.056	15.492	0.929
		30	0.105	-0.021	17.040	0.908
		31	0.056	-0.020	17.485	0.918
		32	0.048	0.015	17.819	0.931
		33	-0.238	-0.156	26.238	0.613
		34	-0.093	-0.010	27.543	0.595

Fig. 12: Correlogram of residuals.

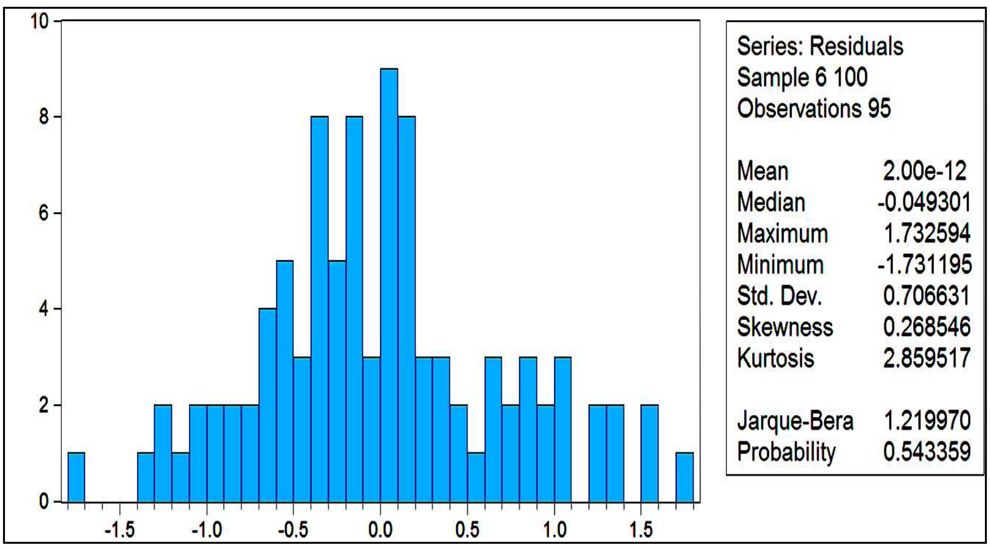


Fig. 13: Normality test histogram.

percentage level of significance. Thus, the null hypothesis is accepted as that the residuals follow a normal distribution. The mean value is also very close to zero. Hence, the identified AR (4) model is very much suitable for forecast.

Forecast

NO_2 concentration has been increasing day by day because of increased vehicular activities. Hence, it is vital to measure the concentration of pollutants in order to mitigate them. Forecasting plays an outstanding role in developing strategies and policies to reduce the amount of primary and secondary pollutants. In this study, we have carried out a short-term static forecast to test the capability of the model. Table 2 displays the results of the forecast.

Table 2: Measured and forecasted values.

S.No	Actual value	Forecasted Value	Residuals
1.	3.72655	3.661018	-0.06553
2.	3.385	4.177981	0.792981
3.	6.4145	4.790519	-1.62398
4.	5.1275	5.063513	-0.06399
5.	3.625	4.184011	0.559011
6.	4.115086	3.93136	-0.18373
7.	3.98877	4.258823	0.270053
8.	5.57635	5.380297	-0.19605
9.	5.578752	4.713327	-0.86543
10.	4.371929	4.285547	-0.08638
11.	4.230024	4.372855	0.142831
12.	4.573359	4.489647	-0.08371
13.	4.941783	5.220355	0.278572
14.	5.411842	5.05643	-0.35541
15.	6.039253	4.589683	-1.44957
16.	5.787678	4.764763	-1.02292
17.	5.899204	5.058178	-0.84103
18.	5.156884	5.348773	0.191889
19.	4.230024	5.587653	1.357629
20.	4.573359	5.60446	1.031101
	Average forecasted error		-0.11068
	Average Absolute error		0.573089

From Table 2, it is evident that the residuals are very small, and they are within ±1.8 deviations. The average forecast error is nearer to zero, which again confirms that the model is satisfactory. The Annual variation of NO_2 concentration shows an increasing trend from the year 2021 to 2022 and is depicted in Fig. 14.

CONCLUSION

An autoregressive model was employed to predict a short-term variation of the daily average NO_2 concentration measured at Nagercoil, India. Out of various models identified from the correlogram plots, the AR (4) model was chosen because of minimum AIC and SC values.NO_2 concentration showed a clear diurnal pattern with two peaks and a minimum value during afternoon hours. The residuals were within the critical limit and were white noise. The Jarque-Bera test followed a normal distribution, and the mean value was very close to zero (2.0e12). Prior to the results obtained from the tests, the AR (4) model was used to forecast the NO_2 concentration. The residuals between forecasted with measured values are very small, and they are within ±1.8 deviations. Also, the average forecast error is nearer to zero, which again confirms that the selected model is very suitable for this study.

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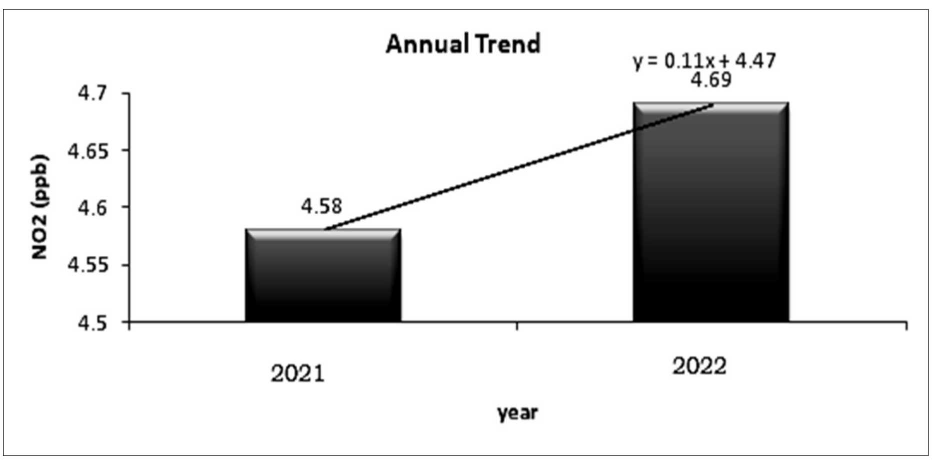

Fig. 14: Annual variation.

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