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Time Series Simulation and Forecasting of Air Quality Using In-situ and Satellite-Based Observations Over an Urban Region

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ABSTRACT

Air quality is directly associated with the health of society. So, it becomes essential to forecast air pollution, which assumes an imperative part in air pollution warnings and control. A time-series simulation approach was adapted for the forecasting of monthly mean ambient air pollutants ($PM_{2.5}$, O_3, NO_2) concentration and Aerosol Optical Depth (AOD) at an urban traffic site (Mathura Road, CSIR-CRRI) in New Delhi, India. Satellite-based aerosol loading (AOD_{550}) retrieved from the Terra MODIS (Collection 6) enhanced Deep Blue (DB) algorithm was used for further analysis. The analysis considered the average monthly mean concentration of air pollutants and AOD between 2012-2017 and, simulates the concentrations of $PM_{2.5}$, O_3, NO_2, and AOD for the same period and then forecasts air quality for the years 2020-2023. The forecasted results were validated with 24 months of in-situ and satellite data from 2018-to and 2019. In the year 2020, observed and simulated results are in lower agreement due to the shutdown of anthropogenic activities to combat pandemic situations. Otherwise, modeled and forecasted results are in good harmony with the in-situ and satellite observations. The results also signify that the time series Autoregressive Integrated Moving Average (ARIMA) modeling approach can be an effective and simple tool for air pollution simulation and future forecast. The results are evocative concerning the forecast of near future aerosol loading information and will also be profound to address the problems.

INTRODUCTION

Indian cities are the epicenter of economic activity and are also on the front lines of some of the world's worst air quality (Choudhary & Gokhale 2016, 2019). Industrialization and unchecked population growth have resulted in increased resource consumption, further amplifying the problem of air pollution (Kumar et al. 2021, Pratap et al. 2020, Choudhary et al. 2020). Millions of casualties happened worldwide because of the worst air quality (Pandey et al. 2021). Air pollution remains one of the most important public health concerns across the globe for the last two decades, contributing to substantial premature mortality with a greater impact in developing nations (Balakrishnan et al. 2019). It is, therefore, important to provide time-to-time air quality forecasts at global, regional, and local scales to support public health authorities (Maji et al. 2021) and policy-makers and enable them to take timely preventative action (Jia et al. 2020) in the short term, long term and event-specific scenarios (Vadrevu et al. 2020) to combat the atmospheric pollutions (Kumar et al. 2018).

In India, geographical boundaries are also favorable and supportive of deteriorating air quality. It is observed in the post-monsoon and winter seasons (October to November and December to February) (Kumar et al. 2020c, Prabhu et al. 2019). Despite this, some episodic events are also well known in India that lead to extremely poor air quality in a particular period of the year (Kumar et al. 2019, 2020a). For example, the rice-wheat crop buildup consumption (CRB) happens two times every year, in April–May wheat crop/Ravi crop and October–November rice crop/Kharif crop, respectively. These periods worsen air quality in many Indian cities (Sarkar et al. 2018). Post-monsoon (October-November) period in India has other episodic events (such as Diwali and biomass burning), and adverse meteorology worsens the air quality. Diwali is associated with burning fire crackers in bulk (Singh et al. 2010) and massive crop residue burning increases the immense load on the local atmosphere. Faiz &Sturm (2000) have assessed that about 10% of respiratory ailments out of thousands of detailed cases are related to climatic contamination every year during these episodic events in Delhi. The Diwali episode lifts PM_{10} and total suspended particulate concentration two to three times in Hisar city, India (Ravindra et al. 2019). Likewise, Barman et al. (2008) additionally revealed that an episodic event Diwali increases pollutants PM_{10}, SO_2, and NO_x concentrations 5.7, 6.6, and 2.7 times, respectively, in contrast to any regular day in Lucknow, India.

In the year 2020 to prevent the COVID-19 transmission, a worldwide lockdown was announced at a different time of the year, and the lockdown imprints were observed in the ambient atmosphere (Kumar et al. 2020b). In India, additionally, air contamination levels dropped altogether with the inconvenience of the 21-day lockdown. To understand the response to complete lockdown, many scientific reports were published to demonstrate the different aspects of air quality all about changes (Chen et al. 2020, Muhammad et al. 2020, Tobíaset al. 2020, Xu et al. 2020). A significant decrease in $PM_{2.5}$, NO_2, and CO concentration before and after lockdown (21-days) were reported by Srivastava et al. (2020) for two Indian cities. Kotnala et al. (2020) stated a 14-time reduction in NO_x concentration (342 to 24 ppb) in New Delhi during the lockdown.

Forecasting, in all aspects, is always very important to formulate the policies to control the situation and condition. Time series analysis is widely implied over the long-term data for comparative analysis and predicts current trends and future forecasts (Soni et al. 2015). The utilization of time series examination depends on the idea that there are some interior trends and patterns inside the data, for example, autocorrelation, patterns, or occasional variety. Several analyses applied the time-series approach to address the air quality by utilizing autoregressive, moving normal models and a mingle of both, known as an autoregressive integrated moving average (ARIMA) (Abish & Mohana 2013, Soni et al. 2014). ARIMA stays as the mainstream model these days due to its adaptability in addressing various sorts of time arrangements, autoregressive (AR), moving normal (MA), and autoregressive moving normal model (ARIMA), it can be defined as ARIMA (p, d, q). When the dataset is non-stationary, the difference will take part in stationary data (AbdRahman et al. 2013). The three stages viz. distinguish verification; assessment and analytic checking assure the precision of time series outcomes (Kumar et al. 2018). ARIMA depends on the Box–Jenkins approach; it is broadly applied in air quality investigations (Box & Jenkins 1976). The insights concerning the ARIMA depicted else ware (McBerthouex & Brown 2002). For time series examination, around 50-100 data points are required (Box & Jenkins 1976, Milionis & Davies 1994). Several researchers considering the impact of meteorological components and apply ARIMA models to anticipate submicron molecule fixations (Jian et al. 2012), day-by-day normal PM_{10} focuses (Liu 2009), and ozone fixation in metropolitan and provincial territories (Duen˜as et al. 2005).

The ARIMA model has widespread application due to its flexibility (Lai et al. 2019, Li et al. 2020, Singh et al. 2020). Therefore, this study's main objectives were as follows, 1) to forecast the future trend of pollutants ($PM_{2.5}$, O_3, and NO_2) and AOD, just after the pandemic episode by applying the ARIMA tool, and 2) to perform a comparative analysis of measured and simulated observations, 3) validation of forecasted results with 25% data (monthly mean of the year 2018-2019, 24 points). 4) Further study will also characterize the trends and variability of the year 2020, emphasizing the lockdown period.

MATERIALS AND METHODS

Data Source

A stationary stochastic ARIMA modeling approach was applied to forecast the monthly mean concentration of ambient air pollutants ($PM_{2.5}$, O_3, and NO_2) and AOD for the urban area of New Delhi, India. The part of data (from 2012-2017) of air pollutants ($PM_{2.5}$, O_3, and NO_2) have been obtained from the automated installed station at CSIR-Central Road Research Institute (CRRI), New Delhi and part of data obtained from CPCB (Central Pollution Control Board) India, for the CSIR-CRRI, New Delhi station for the year 2018-2020. The aerosol optical depth (AOD) at 550 nm was extracted daily for the period 2012 to 2020, from MODIS onboard the Terra satellite for the stations CSIR-CRRI (28.5517° N, 77.2750° E). MODIS measures spectral radiances from 0.55 µm for land with a resolution of 0.1° × 0.1° (https://earthobservatory.nasa.gov/global-maps). The MODIS (Collection 6) enhanced Deep Blue (DB) AOD (Deep_Blue_Aerosol_Optical_Depth_550_Land_Best_Estimate) of level 2, was used in this study. The 24-h average time series data of ambient air pollutants ($PM_{2.5}$, O_3, and NO_2) were averaged into monthly data, similarly daily AOD data were also averaged into monthly AOD then applied the ARIMA for the further analysis.

Quality Control Approach

For quality affirmation, the study used two strategies: (i) outlier recognition and gap-filling procedures were applied to improve the nature of the dataset (Jesus et al. 2020), and (ii) a manual exclusion of zero, negative and invalid information, after reviewing of the dataset. This was applied for the AOD dataset since missing values were greater than those applied for the AOD dataset since missing values were greater than the 365 data points (around 11% of total data). The pollutants $PM_{2.5}$, O_3, and NO_2 have less than 1% missing values for the total assessment period since the gap-filling techniques are generally recommended when missing information rates are more prominent than 5% (Ottosen & Kumar 2019, Junger & De Leon 2015). Therefore, pollutants $PM_{2.5}$, O_3, and NO_2 were manually cleaned and used for the data analysis and interpretations.

Time Series Approach: ARIMA

The ARIMA is a time series simulation method presented by Box & Jenkins in the 1970s and was applied for the current and near-future forecast of the aerosol load to the atmosphere (Kantz & Schreider 1997). Time-series data of the simulation object are considered a stochastic sequence, and this sequence is fitted with some numerical models. When the model is recognized, the future qualities can be anticipated over a wide time period (Kucharski et al. 2020). ARIMA can be defined as ARIMA (p, d, q), a model can be partitioned into three sorts, details are given else were (Kumar et al. 2015). The ARIMA model can discover the qualities and patterns of the time-series information and speculate the future behavior effectively (Kumar et al. 2018).

The time series ARIMA approach was applied to assess the air quality trend before and after the Pandemic episode and the near future air pollutants forecast. The section first portrays the 2012-2017 monthly variation of selected pollutants, section two is characterizing the pollutants' behavior of the year 2020 (Pandemic year), section three is demonstrating the ARIMA simulation and forecasted results, further comparative interpretation of measured, simulated results, and validation data, forecasted observations were described. Such figures are particularly useful in outlining proper approaches for air quality administration (Kumar et al. 2018). The monthly data for the year 2012-2017 (total of 72 data points, 75% of data) was used for the simulation, and monthly data for the year 2018-2019 (25% of data) was used for the validation of the forecasted results (Kumar & Jain, 2009). The extraction and assessment of model boundaries are accomplished by utilizing the ARIMA by using the SPSS package. Different criteria were used to evaluate the model fits and goodness, explained else were (Gocheva-Ilieva et al. 2014).

RESULTS AND DISCUSSION

Year to Year Variation of Pollutants

Fig. 1 demonstrates the monthly variation of pollutants $PM_{2.5}$, O_3, NO_2, and AOD for the period 2012 to 2017. The cyclic and seasonality patterns are very distinct in the figure, particularly for the $PM_{2.5}$ and AOD (Kumar et al. 2019, 2020a). Highest emission peaks observed for post-monsoon period (October-November, as per Fig. 1 post-monsoon months are: 10-11, 23-24, 35-36, 47-48, 59-60, 71-72). In the monsoon season, pollutants concentration drops to a minimum, the dropping peaks are also very apparent corresponding to the monsoon season (July-September, as per Fig. 1 monsoon months are: 7-9, 19-21, 31-33, 43-45, 55-57, 67-69). The O_3 and NO_2 also follow the cyclic seasonality trend, but the peaks get flattened with the proceeding years.

The descriptive statics of the data is depicted in Table 1. The higher skewness value (0.695 to 1.5) indicates that data are in non-symmetrical distribution. Likewise, the kurtosis ranges of 0.511 to 2.97 indicate leptokurtic distribution. The time series simulation approach, ARIMA was applied to the 2012-2017 (75% of data) data set for the future forecast. It was also observed from the data that $PM_{2.5}$ concentrations are much higher (greater than double of NAAQS limit) as compared to NAAQS annual limit (40 $\mu g.m^{-3}$) whereas the annual concentration of NO_2 and O_3 concentration is double the annual and 8-hourly NAAQS limit (19.48 ppb, 46.69 ppb), respectively.

Pollutants Trend in 2020

To break the transmission of COVID-19 worldwide, the lockdown was forced at a different time in 2020. In India, the Government deployed a complete lockdown that

Table 1: Descriptive statistics of air pollutants.

Variables	Observations (N)	Minimum	Maximum	Mean	Skewness	Kurtosis
$PM_{2.5}$	67	16.76	295.20	111.58	0.82	1.21
NO_2	67	5.12	123.92	42.03	1.50	2.95
O_3	66	23.81	134.05	63.12	0.70	0.53
AOD_{550}	71	0.42	1.56	0.82	0.87	0.51

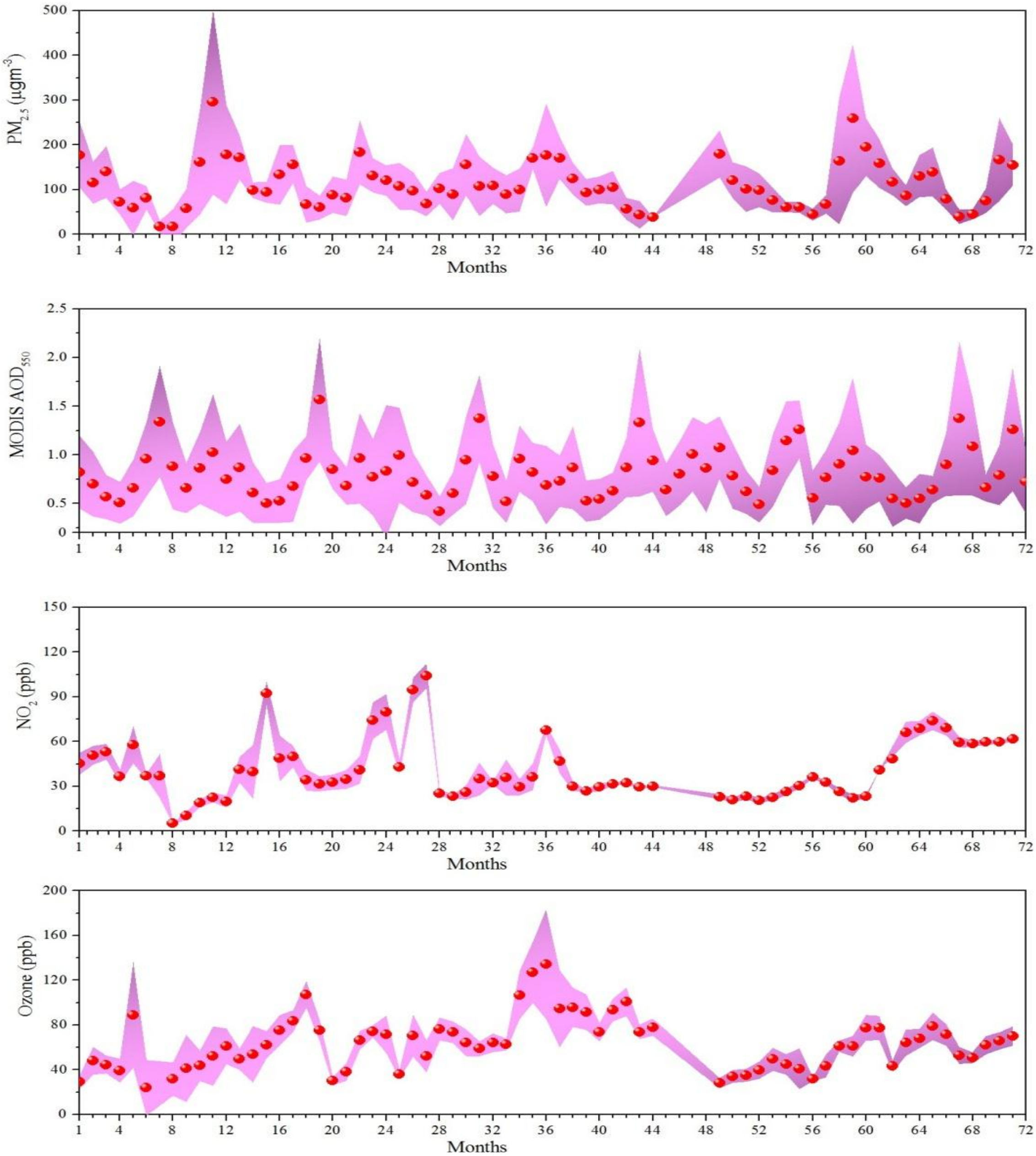

Fig. 1: The monthly variation of pollutants $PM_{2.5,}$ AOD, NO_2, and O_3 for 2012-2017.

stopped all the anthropogenic activities, which are the main source of air pollution in the atmosphere. Numerous published researches explained air quality with respect to lockdown (Kumar et al. 2020b). Indian government deployed complete lockdown for 21 days from 25th March, then slowly released the term and condition of lockdown until 31st May 2020. Therefore, very sharp drops in pollutants concentration were observed during 21 days of complete lockdown. Fig. 2 depicted the trend of pollutants and AOD in the year 2020, the lockdown period is highlighted as yellow. After the lockdown period, due to the monsoon season wash-out, significant pollutant concentration drops were observed. The average concentration of the pollutants $PM_{2.5}$, NO_2, $O_{3,}$ and AOD in the year 2020 was found as 88.77±74 μg.m^{-3}; 38.40±29.40 ppb; 18.40±9.12 ppb and 0.73±0.45, respectively. The maximum concentration is

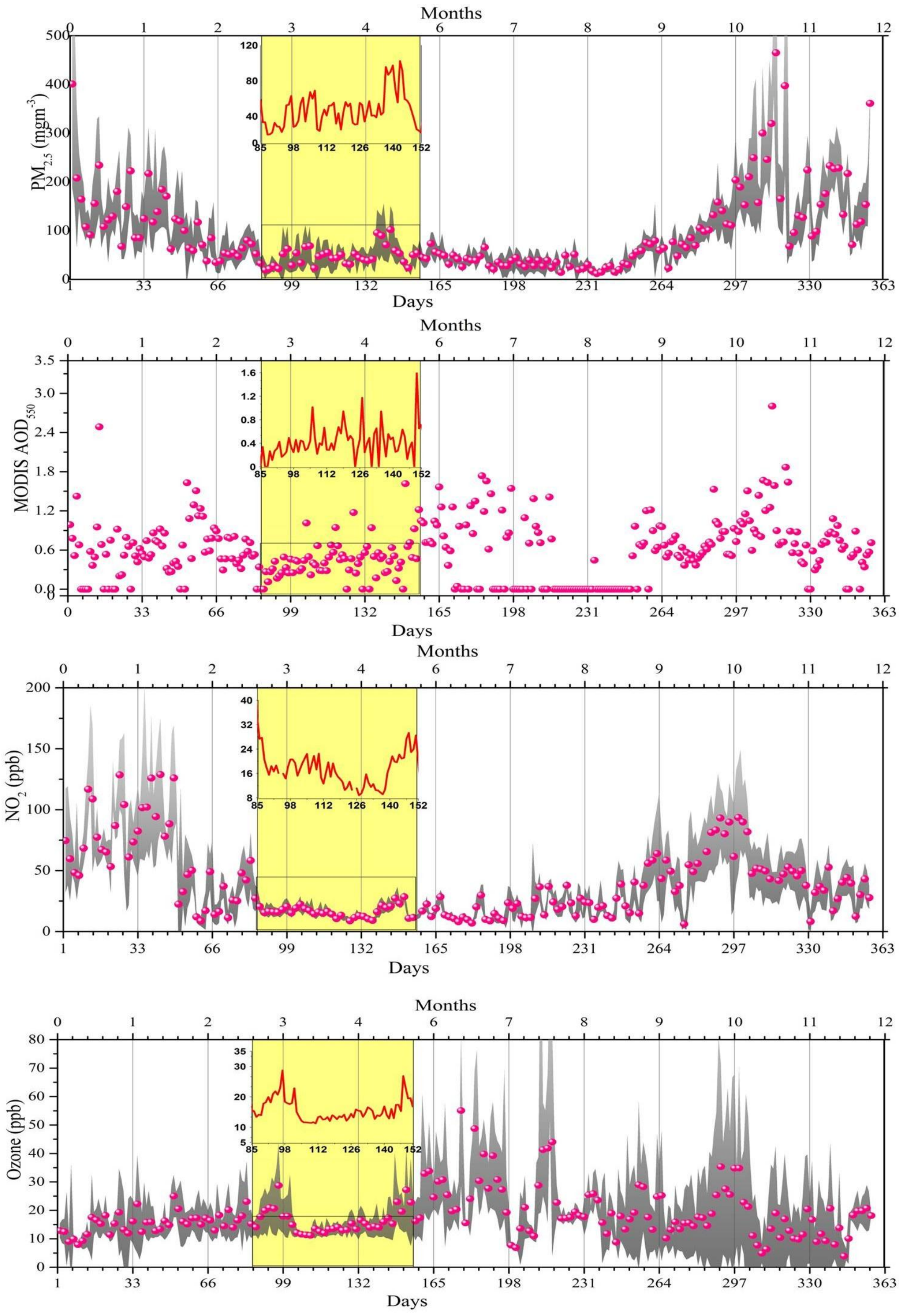

Fig. 2: Daily-based trend of $PM_{2.5}$, MODIS AOD_{550}, NO_2, and O_3 during 2020, the lockdown period is highlighted as yellow.

reported as 473.92 µg.m^{-3}, 151.27ppb, 82.84 ppb; 2.80 for $PM_{2.5}$, NO_2, O_3 and AOD, respectively, and minimum concentration of $PM_{2.5}$, NO_2, O_3 and AOD is 12.05 µg.m^{-3}, 6.18 ppb, 3.90 ppb and 0.66, respectively. The lockdown duration average concentration was 46.65±23.42 µg.m^{-3}, 16.58±3.63 ppb; 15.69±4.41 ppb; and 0.46, respectively. The maximum lockdown concentration of $PM_{2.5}$, NO_2, O_3 and AOD was 102.23 µg.m^{-3}, 29.32 ppb, 28.72 ppb, and 1.62, respectively and minimum lockdown concentrations were reported as 19.22 µg.m^{-3}, 8.85 ppb, 11.22 ppb and 0.11, respectively.

The data are presented in Table 2 for a better relative overview. The pre-lockdown and lockdown pollutants concentration demonstrated that the concentration of the selected pollutant drops to half as compared to the past 9 years' concentration, except for AOD. In case AOD magnitude drops are around 25%.

Time Series Simulation and Forecast

The ARIMA model was applied for simulation and forecasting pollutants concentration ($PM_{2.5}$, NO_2, and O_3) and MODIS AOD for CSIR-CRRI, Delhi-Mathura Road, urban area, New Delhi. The analysis considered the monthly average concentration of pollutants and AOD for 2012-2017 and simulated the monthly concentration of pollutants and AOD and forecast the pollutants and AOD for the period of forecast the pollutants AOD for 2020-2023. The large variations in $PM_{2.5}$ values moderate variations in MODIS AOD; however, low variations were found in NO_2 and O_3 values (Fig. 3). The observed and simulated values of pollutants and AOD are lies within the upper control limit (UCL) and lower control limit (LCL) boundary, indicating a satisfactory agreement between in-situ measurement and ARIMA-based simulations.

The measured and simulated observation trends for air pollutants ($PM_{2.5}$, NO_2, and O_3) and MODIS AOD_{550} are found in good agreement, as depicted in Fig. 4. It is clearly shown that the monthly AOD values are found higher during pre-monsoon (May to June) and decreasing during monsoon (July to September) and again, increasing trends occur during post-monsoon (October to November) and winter (December to February) months, of almost every year. However, higher concentrations of $PM_{2.5}$ were found during post-monsoon mainly due to biomass burning transported from the Punjab and Haryana states and during winter months due to transportation, biomass/wood burning, and fog.

Fig. 5 depicts the trends of the residuals ACF and PACF, demonstrating that all points are randomly distributed, and suggesting that model outcomes are satisfactory. Also, each pollutant's residual autocorrelations are small and are within the significance bounds limit.

The statistical significance of the model was evaluated by Normalized Bayesian Information Criterion (BIC), the R–square, Root Mean Square Error (RMSE), Mean Absolute Percentage Error (MAPE), Mean Absolute Error (MAE), and Ljung – Box Q statistic were used to test for the adequacy and statistical appropriateness of the model. The Ljung–Box Statistic of the model values for Normalized BIC lies between -4.393 to 7.062 for the 16 degrees of freedom (Table 3).

The stationary-R^2 also depicts the good fit between observed and simulated values. ARIMA performed better for $PM_{2.5}$ (0.752) and NO_2, a lower value of R^2 indicates moderate fit (R^2: 0.585) as compared to other pollutants.

Table 2: Overview of the pre-lockdown period, lockdown year, and lockdown period.

Variables		Pre-lockdown (2012-2017)	Lockdown year 2020	Lockdown period of 2020
AOD	Avg	0.60 ±0.05	0.73±0.45	0.46±.26
	Max	1.54	2.80	1.62
	Min	0.21	0.66	0.11
$PM_{2.5}$	Avg	111.58±53.69	88.77±74	46.65±19.9
	Max	295.76	473.92	102.23
	Min	16.2	12.05	19.22
NO_2	Avg	13.93±3.40	38.40±29.40	16.58±4.82
	Max	21.37	151.27	29.32
	Min	9.62	6.18	8.85
O_3	Avg	33.92±16.81	18.40±9.12	15.69±3.70
	Max	76.45	82.84	28.72
	Min	12.14	3.90	11.22

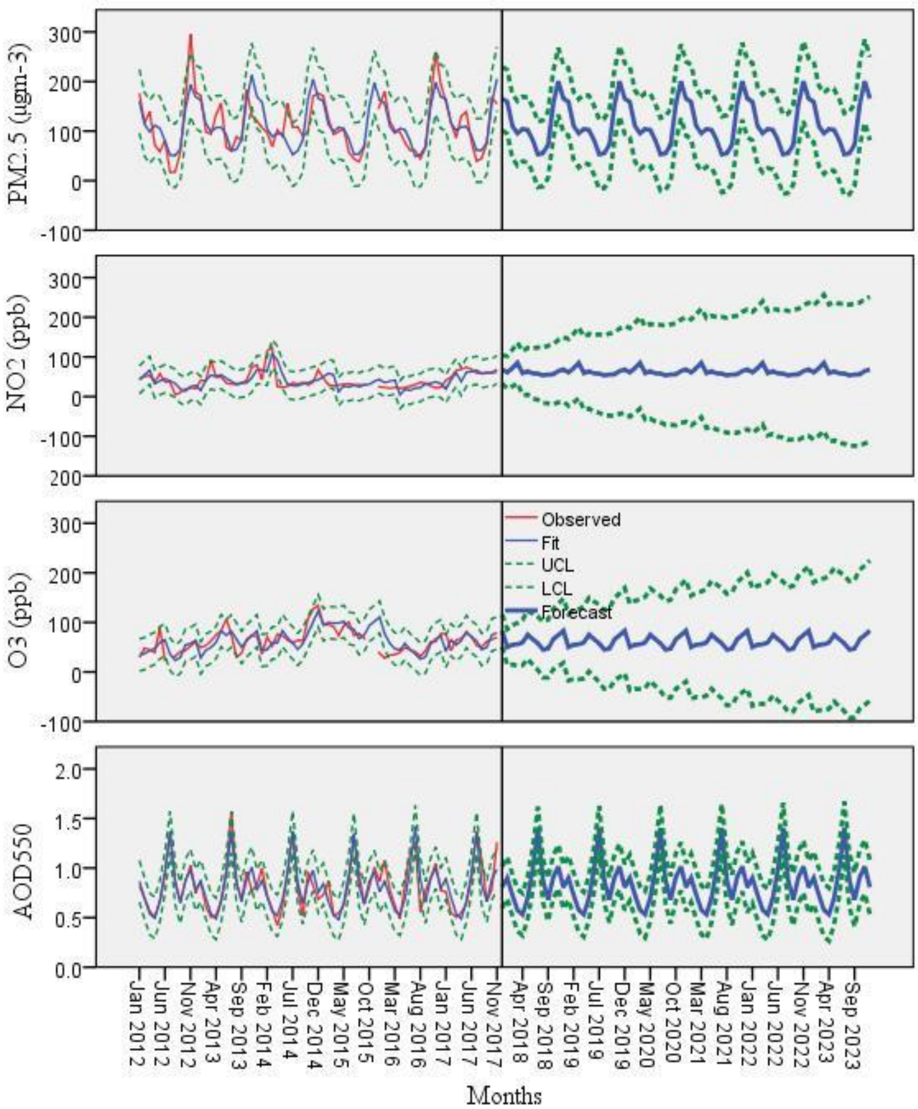

Fig. 3: Comparison of ARIMA model simulations and forecasting (blue line) with observed $PM_{2.5}$, NO_2, O_3, and MODIS AOD_{550} (red line).

The more or less similar values of the stationary-R^2 and the R^2 of all selected pollutants and AOD are indicating that the simulated model is reasonably good. Model fit statistics is given in Table 4.

The lower RMSE values (ranges of 0.105-32.084) between observed and simulated pollutants and AODs for a period of 2012-2017 are supportive of favorable results. The MAPE values are ranging 20-to 50, also indicating the

Table 3: Ljung Box statistics.

Normalized BIC	Statistic	DF	Sig.
7.062	52.938	16	0.000
5.869	54.806	16	0.000
5.703	34.432	16	0.005
-4.393	23.177	16	0.109

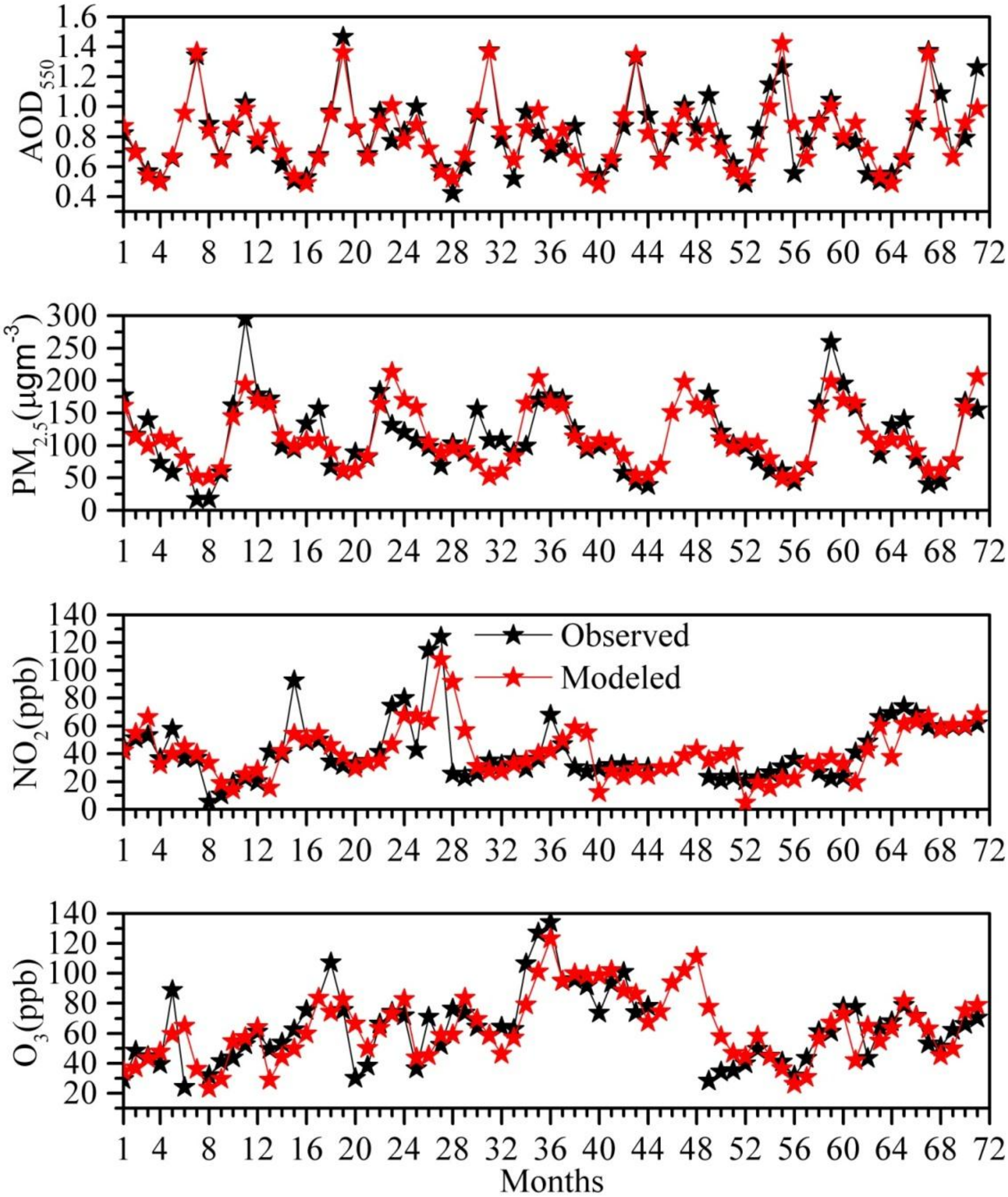

Fig. 4: Comparison of observed and simulated results of $PM_{2.5}$, NO_2, O_3, and MODIS AOD_{550}.

reasonability of the fitted model (Delurgio 1998). This indicates that the model has adequately captured the correlation in the time series.

The 24 months data for the year 2018-2019 were used for the validation of forecasted results. The obtained forecasts for the next 48 months (2020-2023) are also excellent compared to actual observations other than those used in the model, retaining the same trend. The forecasted results were (48 months in the year 2020-2023) validated with measured observation (2018-2019, 24 data points) showing an agreeable association, as depicted in Fig. 6.

In Fig. 6, the year 2020 measure and simulated observations were also compared to know the difference between the pandemic year pollutants concentration and the regular data-based simulated value. The year 2020 has different trends of pollutants due to pandemic conditions. It is identified that there is a significant difference in magnitude of the pollutants, but the variable behavior remains the same

Table 4: Model Fit Statistics.

Variables	Stationary R-squared	R-squared	RMSE	MAPE	MAE	t-value	p-value
$PM_{2.5}$	0.752	0.648	32.084	26.522	22.961	1.321	0.1025
NO_2	0.585	0.383	17.672	41.479	12.253	4.813	0.0000
O_3	0.700	0.537	16.246	23.850	12.065	4.709	0.0001
AOD_{550}	0.744	0.824	0.105	9.236	0.073	1.290	0.1076

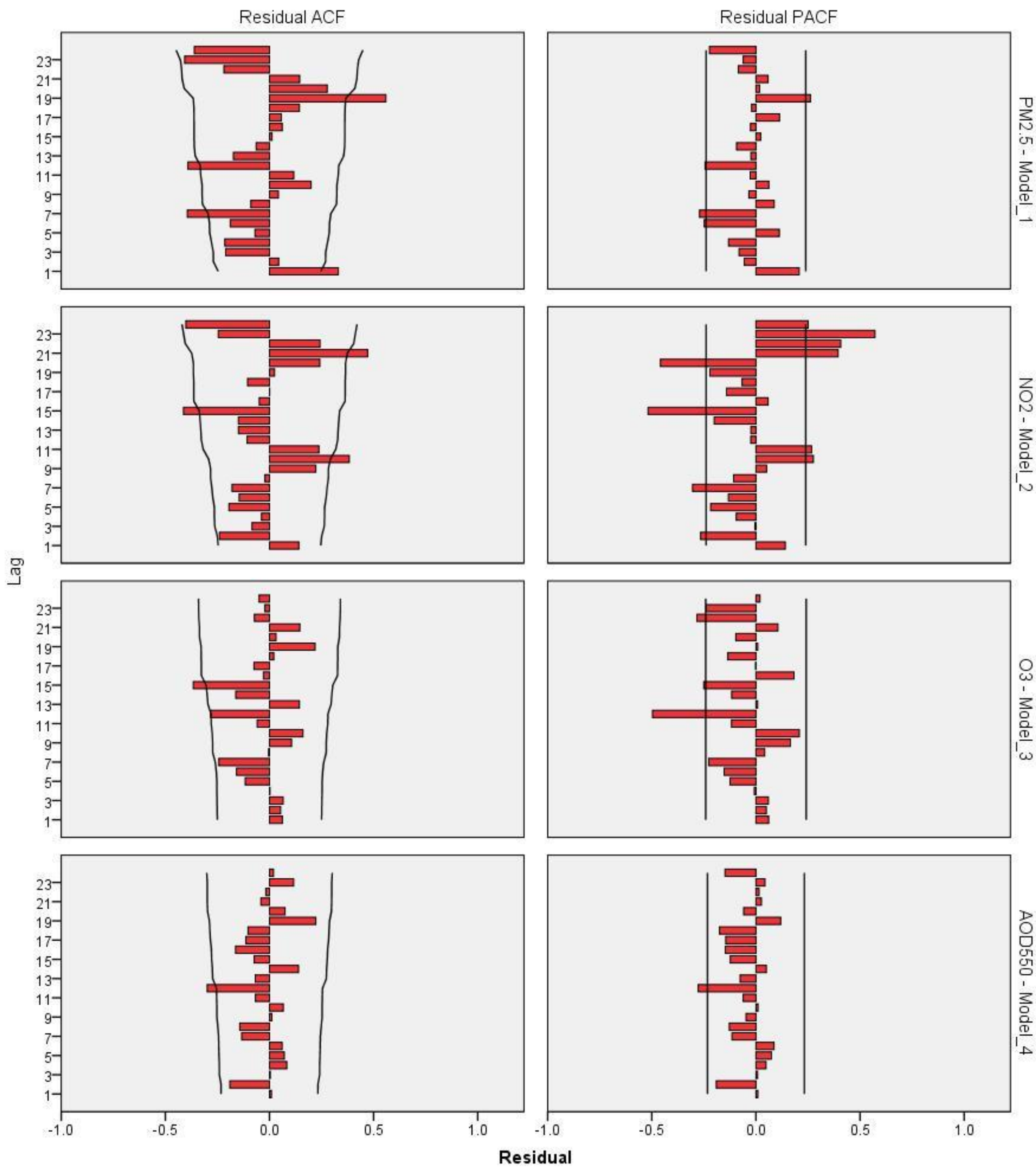

Fig. 5: Residuals of ACF and PACF for the selected modelsofPM$_{2.5}$, NO_2, $O_{3,}$ and MODIS AOD$_{550}$.

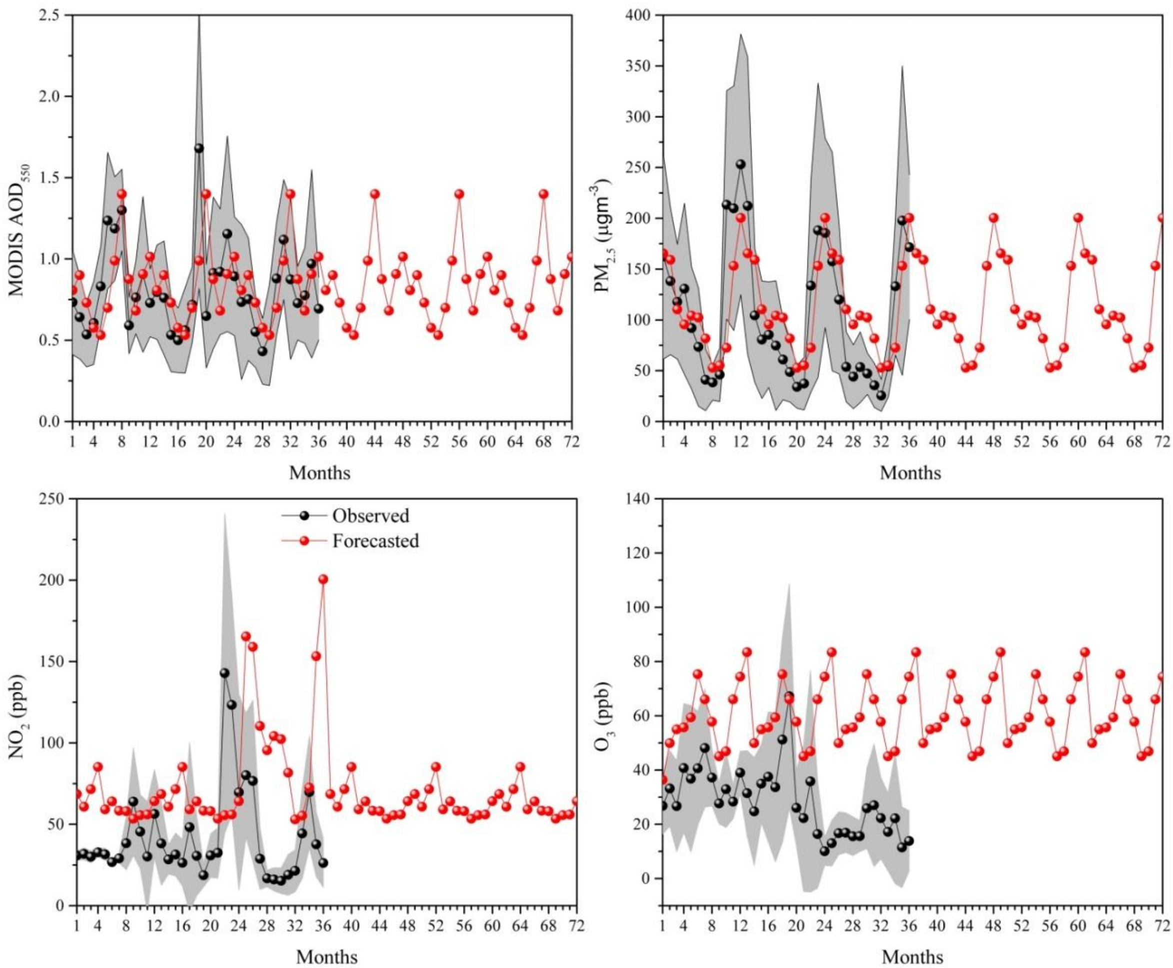

Fig. 6: Validation of modeled $PM_{2.5}$, NO_2, O_3, and MODIS AOD_{550} with observed $PM_{2.5}$, NO_2, O_3, and MODIS AOD_{550}.

in the case of $PM_{2.5}$ and AOD whereas, O_3 and NO_2 have slightly different trends in contrast to a regular pattern. Based on the collective assessment of the model output, ARIMA simulation and forecasting results were found consistent. However, unpredictable meteorology and heterogeneity in the aerosol optical properties bring limitations in the model's output, for example, moderate to low performance of ozone concentrations might be due to these limitations (as observed in Fig. 6 for ozone concentration).

CONCLUSION

The data statics demonstrated the non-symmetrical data and leptokurtic distribution of pollutants $PM_{2.5}$, O_3, NO_2, and AOD from 2012 to 2017. The pre-lockdown and lockdown comparative analysis demonstrate that in the year 2020, except for AOD, pollutants concentration decreased to half in magnitude compared to the past nine years' concentration. The simulated and forecasted result shows good agreement with the observed and validation data. Different model fit statics, and the five accuracy measures criteria also demonstrated the harmony of results. In the context of air quality management, the ARIMA-based prediction demonstrates better suitability for the MODIS AOD, $PM_{2.5}$, and NO_2 as compared to the O_3 at an urban location in New Delhi. ARIMA approach, in combination with satellite data, can be a good option to forecast future aerosol load for areas where the ground data is a major limitation for the research.

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