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Estimation of Particulate Matter ($PM_{2.5}$) Over Kolkata

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Abstract—Particulate matter has a diverse range of effects on human health and climate due to which it has emerged as a key parameter in monitoring air quality. The current study explores and estimate the concentration of particulate matter ($PM_{2.5}$) from MODIS AOD product over the city of Kolkata for a period of 3 years (2019–2021). $PM_{2.5}$ concentration dataset was acquired from seven CPCB ground stations spread throughout Kolkata. Further, the study utilized the 1-km MODIS AOD product and meteorological parameters from MERRA-2. Considering the statistical analysis of data, four regression models were derived and considered for PM estimation. Daily estimated $PM_{2.5}$ concentrations were compared against respective observations. The developed models were evaluated with the help of statistical methods. Model-2 based on the multi-linear regression equation was found to be the best fit model having a strong positive correlation between the estimated and observed $PM_{2.5}$ values (R = 0.814). The root mean square error (RMSE) was estimated at 22.54 $\mu g/m^3$. The estimated $PM_{2.5}$ values were able to capture the trend of $PM_{2.5}$ concentrations on the ground level. The normalized mean bias (NMB) value was − 0.315 and the mean absolute error was 18.94. The mean absolute percent error is estimated at around 5.16%. The results demonstrated that the developed model thus can be used to study the particulate matter concentration over areas where ground-based observation sites are sparse on the city level.

Keywords: Particulate Matter, AOD, Regression Model, $PM_{2.5}$.

1. Introduction

In the recent decade, air pollution has emerged as a matter of critical concern, especially for the major urban centres of the world. It not only threatens public welfare and human health, but also the world's climatic system. From disturbing the hydrological cycle to increasing the globe's temperature, air pollution is known to impart an array of negative impacts (Satheesh & Ramanathan, 2000; Singh et al., 2020; Wang et al., 2014). Additionally, air pollution is a major health risk (Sathe et al., 2019) holding the fourth highest rank in mortality risk factor and was responsible for 12% of deaths globally in 2019 (Brauer et al., 2021). Inhabiting about 80% of the world's population, developing nations that are middle to low-income in economy report 90% of diseases and fatalities due to air pollution (Sathe et al., 2019; WHO, 2016). Air pollution is a dynamically complex mixture that primarily comprises both particulates and gaseous compounds having different sources of emission; majorly transport and industrial sectors (Badami, 2005; CPCB, 2010; Gulia et al., 2015; Sathe et al., 2019) and with space and time these pollutants undergo transformation processes (Brauer et al., 2021). One of the major subset of air pollution is Particulate Matter (PM), a major pollutant in cities, which is airborne solid or liquid particles smaller than 2.5 µm in aerodynamic diameter ($PM_{2.5}$). The negative effects of $PM_{2.5}$ on both the climatic system and public health are well documented in the literature (Brauer et al., 2021; Hanzalova et al., 2010; Sathe et al., 2019; Satheesh & Ramanathan, 2000; Singh et al., 2020; Valavanidis et al., 2008; Wang et al., 2014; WHO, 2016). Numerous epidemiological studies have demonstrated the association of $PM_{2.5}$ with adverse human health effects, such as cardiovascular and respiratory diseases (Donkelaar et al., 2010; Lim et al., 2011; See & Balasubramanian, 2008; Song et al., 2014).

Due to its effect on human health and climate hence the environment, $PM_{2.5}$ has become a key

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parameter in monitoring air quality (Fuzzi et al., 2015; Kim et al., 2015; Tuygun et al., 2021). The measurement of $PM_{2.5}$ concentrations at ground level is therefore very important to adequately address the aforementioned concerns. In general, the concentration dataset acquired from ground-based stationary monitoring stations is considered to be the most accurate. However, continuous spatial monitoring is frequently constrained by it's quality, consistency and data frequency (Hu et al., 2013). Additionally, ground instruments tend to be an expensive and impractical choice of data collection if the area of interest is a large city (large spatial coverage) or continuous monitoring is essential (Song et al., 2014; Tuygun et al., 2021). On the contrary, insufficient data on natural sources and inventories of anthropogenic emissions frequently hinder the state-of-the-art air pollution models (Dawson et al., 2007; Koelemeijer et al., 2006; Pelletier et al., 2007; Tian & Chen, 2010). For the assessment of the present-day air dispersion models, air pollution control strategies, and other environmental climate changes; accurate mapping of the air pollutant concentration and its seasonal as well as annual variation assessment is crucial. Therefore, researching the methods of estimation of $PM_{2.5}$ in areas having fewer monitors at a spatial scale is an important approach that is currently being extensively researched.

One such approach is remote sensing technology which has been extensively used in recent years to monitor $PM_{2.5}$ from space (Donkelaar et al., 2006; Jia & Liu, 2006; Liu et al., 2005; Wang & Christopher, 2003). Estimation and assessment of $PM_{2.5}$ concentrations over large areas can be accomplished using satellite-derived aerosol optical depth (AOD). AOD is the integral form extinction i.e., scattering and absorption (Lee et al., 2012) of light (sunlight) by aerosols present in the total vertical air column from the surface of the earth to the top of the atmosphere (Tsai et al., 2011), or in simple terms, exponential attenuation of incident radiation from the sun by particles floating in the atmosphere (Kumar et al., 2007; Tuygun et al., 2021). The Moderate Resolution Imaging Spectroradiometer (MODIS) provides one of the most reliable long-term aerosol data records among several other satellite sensors capable of retrieving AOD. Since March 2000, MODIS—a sensor onboard the NASA satellites "Terra" and "Aqua"—has provided daily AOD data with a nadir resolution of 10 km^2 and has been widely used to estimate ground-level $PM_{2.5}$ concentrations. Recently, the Multi-Angle Implementation of Atmospheric Correction (MAIAC) processing algorithm was developed, which downscaled AOD data at 1 km^2 resolution (Lyapustin et al., 2011a, 2011b). For PM estimation, other algorithms that provide 1 km^2 resolution AOD data were also used by the research community. The MODIS-AOD dataset has been used in conjunction with meteorological parameters in several regions around the world to provide reliable daily $PM_{2.5}$ estimates over large spatio-temporal domains. Furthermore, it has recently been validated against PM data in India (Dey et al., 2020; Mhawish et al., 2019), with positive results.

To investigate this quantitative relationship between satellite-derived AOD and ground-measured $PM_{2.5}$ several models have been developed, including the semi-empirical model (Koelemeijer et al., 2006), mixed effects model (Lee et al., 2011; Yap & Hashim, 2013), generalized additive model, general linear and nonlinear regression model (Donkelaar et al., 2010; Liu et al., 2007). To predict PM concentration in urban areas, approximately 30% of studies used a multiple linear regression model (Bera et al., 2021). Furthermore, it was suggested that meteorological factors are to be incorporated into the AOD–$PM_{2.5}$ relationship to improve model performance (Guo et al., 2009; Liu et al., 2009; Tian & Chen, 2010). However, the estimation accuracy of the above models still has space to improve (De Leeuw et al., 2006).

The present paper thus focuses on the simulation of $PM_{2.5}$ concentration at city-scale. Kolkata city was selected as the region of interest. Being the economic growth center of eastern India, Kolkata is one of the ten most polluted cities in India and one of the world's 25 most polluted cities (WHO, 2011). In this study, a multiple linear regression model along with exponential and linear-log models have been used for simulating the $PM_{2.5}$ concentration (2019–2021) at 1 km^2 resolution over Kolkata (approximately 206 sq. km. in the area) considering the unique geo-climate of the city. The objective of present research was to fill a knowledge gap and quantify the shortterm change in $PM_{2.5}$ concentrations using AOD as surrogate over Kolkata (one of the largest agglomerations in the region of North Eastern India). Additionally, the selected study period included a special event of COVID-19 lockdown situation. Therefore, performing a study on estimation of PM under these conditions provide a novel perspective on the model's overall performance and its ability to capture special events.

2. Study Area

Located at 22.5625°N and 88.3531°E in the Indian subcontinent, Kolkata is the capital city of the state of West Bengal. The city is situated at an altitude of ~ 8 m above mean sea level close to the coastline (145 kms away from the sea) of the Bay of Bengal (Dasgupta, et al., 2013; Mangaraj et al., 2022). It is the third most populous metropolis in India spread over an area of ~ 206 sq km and has an extended metropolitan population of over 14.9 million as of 2020 (Mangaraj et al., 2022).

The climate of the city is both wet and dry and it is vulnerable to climatic disasters like flooding, tropical cyclones, tidal upsurge, local storms (kaalbaisakhi), and intense local precipitations (Dasgupta et al., 2013). The mean annual temperature between the years 2019 and 2021 is 25.84 °C (https://power.larc.nasa.gov/, accessed on 8 June 2022). The mean annual temperature is 26.8 °C and annual precipitation is 1600 mm with August being the rainiest month (Dasgupta et al., 2013). Due to the presence of two special geographical features—the rivers Hoogly on its western edge and Kulti-Bidyadhari on its east, the city of Kolkata is a highly urban and commercial settlement and the city spread alongside it in the north–south direction. Figure 1 displays the exact locations of the air quality monitoring stations spread across the city of Kolkata and Table 1 summarises the coordinates of the stations from where the ground data of $PM_{2.5}$ was obtained. The seven-point locations which had the instruments installed and from where the ground observation data was retrieved are Ballygunge, Bidhannagar, Jadhavpur, Fort Williams, Rabindra Bharti University, Rabindra Sarobar, and Victoria Memorial.

3. Materials and Methods

3.1. Data Collection

The study was conducted for a period of 3 years i.e., from 2019 to 2021. The study employs three different types of datasets:

1. Daily averaged combined Moderate Resolution Imaging Spectroradiometer (MODIS) Aqua and Terra AOD data at 550 nm (MCD19A2).
2. Daily $PM_{2.5}$ data (ground-based) from Central Pollution Control Board (CPCB).
3. Meteorological parameters (temperature, relative humidity, and windspeed) acquired from Modern-Era Retrospective analysis for Research and Applications, Version 2 (MERRA-2) platform.

3.1.1 MODIS AOD

The study utilized Level-2 AOD dataset obtained from MODIS satellites over Kolkata, having a spatial resolution of 1000 m and a temporal resolution of 1–2 days. MODIS operates on two satellites: EOS AM-1 TERRA, launched in 1999, and EOS AM-1 AQUA, launched in 2002. TERRA moves from north to south, crossing the equator at 10:30 a.m. IST, whereas AQUA moves from south to north, crossing at 1:30 p.m. IST (Chu et al., 2002; Dey et al., 2012; Kaufman et al., 2002; Lee et al., 2011; Levy et al., 2007; Payra et al., 2015; Remer et al., 2005; Song et al., 2014; Soni et al., 2018; Yap & Hashim, 2013). MODIS has a swath width of 2330 km, orbits at 705 km from Earth, and provides AOD measurements in the visible to thermal infrared spectrum (Lee et al., 2012; Levy et al., 2007; Schaap et al., 2009). The dataset, sourced from NASA's Goddard Earth Sciences Distributed Active Archive Centre, covers 2019–2021. The combined Aqua and Terra MODIS dataset, processed using the MAIAC algorithm, was obtained at a spatial resolution of 1 km (MCD19A2). MAIAC utilizes MODIS time series and a Physical Atmosphere Surface Model, ensuring fewer unknowns than measurements (Chudnovsky et al., 2014). It employs various filters, including cloud screening and adjacency tests, producing accurate results. MAIAC's accuracy was validated against

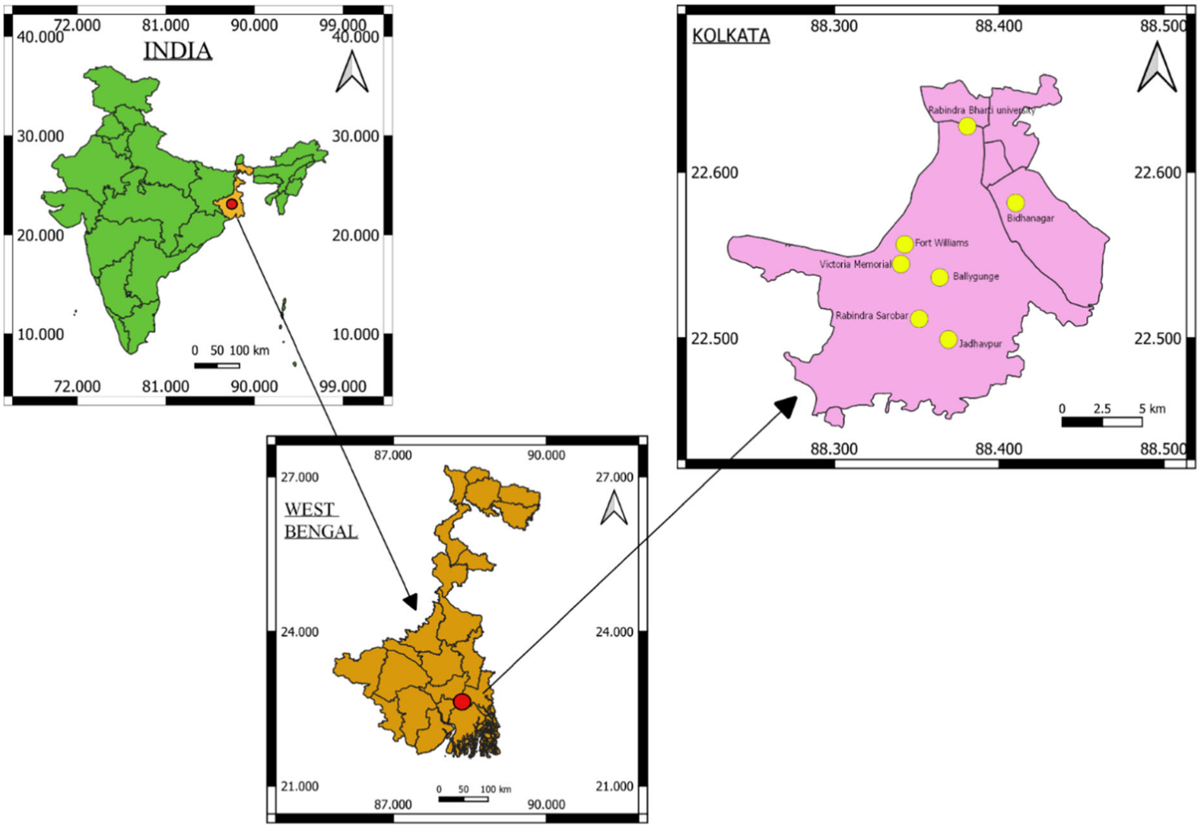

Figure 1
Study area map of Kolkata showing the point locations of CPCB stations

Table 1

Coordinates of the CPCB stations throughout Kolkata

Station ID	Station name	Latitude (°North)	Longitude (°East)
1	Ballygunge	22.4993	88.3692
2	Bidhannagar	22.5117	88.3514
3	Jadhavpur	22.5367	88.3638
4	Fort Williams	22.5448	88.3404
5	Rabindra Bharti University	22.5566	88.3427
6	Rabindra Sarobar	22.5816	88.4100
7	Victoria Memorial	22.6279	88.3801

AERONET data, demonstrating superior performance over urban areas (Lyapustin et al., 2011a, 2011b). The algorithm incorporates a cloud masking technique and provides data at a uniform gridded resolution of 1 km, oversampled by a factor of 2. The combined AOD product from Aqua and Terra was chosen for its enhanced spatio-temporal coverage between 10:00 a.m. and 2:00 p.m., making it representative for the study. The dataset and algorithm details are available at https://ladsweb.nascom.nasa.gov/.

3.1.2 Monitoring Data

Daily $PM_{2.5}$ mass concentration across seven point locations across Kolkata for years 2019–2021 was obtained from the CPCB website (source: http://www.cpcb.gov.in/CAAQM/frmUserAvgReportCriteria.aspx). In India, ground-based $PM_{2.5}$ data is measured by automated instruments and made available publically on the CPCB website. To achieve further spatial coverage, ground-based data of PM is necessary to complement and support figures from a different source as satellite products (Sathe et al., 2019). $PM_{2.5}$ has been measured by CPCB with BAM 1020 which works on the principle of Beta Ray attenuation. The detailed working of the instrument can be found elsewhere (Hama et al., 2020).

3.1.3 Meteorological Data

All the meteorological parameters which were used in the analysis (temperature, relative humidity, and wind speed) was acquired from NASA POWER (at the respective height of 2 m, 2 m, and 10 m), one of the sites of NASA that provides data through MERRA-2 outframe. MERRA-2 was developed by Global Modelling Assimilation Office (GMAO) (Ma et al., 2020; Randles et al., 2017) and uses data assimilation of an upgraded version of Goddard Earth Observing System Model, Version 5 (GEOS-5) of version 5.12.4 (Bosilovich et al., 2016). This version of GEOS uses recently developed microwave sounders and hyperspectral infrared radiance instruments along with other data types. All the data in MERRA-2 is provided at an identical horizontal grid comprising 576 points longitudinally and 361 points latitudinally with a resolution of $0.625° \times 0.5°$ (Bosilovich et al., 2016). The meteorological parameters considered to conduct the study were selected based on the previous research work of Kumar et al. (2007), Kanabkaew (2013), Gupta et al. (2006), Gupta and Christopher (2009), Chitranshi et al. (2015) and Soni et al. (2018). The relationship between AOD and PM also depends upon meteorological factors which are described below and hence supporting the choice of meteorological parameter selection.

a. Temperature: The data for temperature was obtained at 2 m height from the surface and it was considered for it could enhance photochemical reactions between particulate precursors (Soni et al., 2018; Tian & Chen, 2010; Wang & Ogawa, 2015).
b. Relative humidity: Dataset obtained at 2 m height for relative humidity for it can directly have an impact on the size of particles considering the effect of hygroscopic growth (Kumar et al., 2011; Soni et al., 2018).
c. Wind speed: A dataset at 10 m was acquired for its ability to cause advection and turbulent mixing (Kumar et al., 2011; Soni et al., 2018).

3.2. Data Processing and Collocation

Before analyzing the data, the raw data is collected and compiled over the desired location. The MODIS AOD data (MCD19A2) is in Geotiff file format. With the use of the QGIS software Version 2.14, data for each month is extracted for the seven-point locations of Kolkata. Three to four data values are available for one day at each point location. The values are averaged to extract daily values which are again compiled accordingly to derive the annual value of AOD. By matching the dates for which daily values of AOD, $PM_{2.5}$, and the daily meteorological parameters were available, the data compilation was completed.

Controlling the data quality is essential to avoid any errors and increase the reliability of the study. Hence, any AOD values which was given as zero due to noise or error in diagnosis have been excluded from the study realizing the potential of its impact on the dataset and average hence the inference in the study. The same procedure was followed for the $PM_{2.5}$ values. The reason for such ambiguous values present in the $PM_{2.5}$ dataset was the concentration of $PM_{2.5}$ which was beyond the detectable range of the monitors (Sathe et al., 2019). The meteorological data were acquired from MERRA-2, which already gives the processed result for parameters selected by integrating values of the satellite and validating it with the ground data. Again, if any day had any of the parameters missing, that day was eliminated from the study.

The final datasets obtained were then divided into the Modelling and Validation Dataset. Around 1470 point dataset is used for developing regression model for Kolkata that underwent rigorous filtering and calibration to ensure data quality. Missing values in dataset were truncated to handle the missing data, and thus clean dataset was used for developing a regression model. Validation is also done over the same study area but for a month (217 data points) to avoid autocorrelation during validation and evaluation of regression models. The aim of the study is to assess the overall performance of PM model over city (Kolkata) scale. There is limitation of less data availability during the monsoon season. Therefore, cross-validation techniques have been employed.

This ensured that the limited monsoon data is represented in various validation folds monthly. Figure 2 describes the methodology followed for the estimation of $PM_{2.5}$ concentration.

3.3. Model Description

To estimate $PM_{2.5}$ from MODIS AOD and various meteorological parameters, different model Eqs. (1–4) were derived. The efficiency of all derived models are compared to achieve the best fit model for estimation of $PM_{2.5}$ concentration over Kolkata.

3.3.1 Model 1

This model uses only two parameters which are: MODIS AOD and $PM_{2.5}$ from CPCB and assumes a linear relationship among them. This is a preliminary model and does not consider any other values or governing parameters affecting PM concentration at any location.

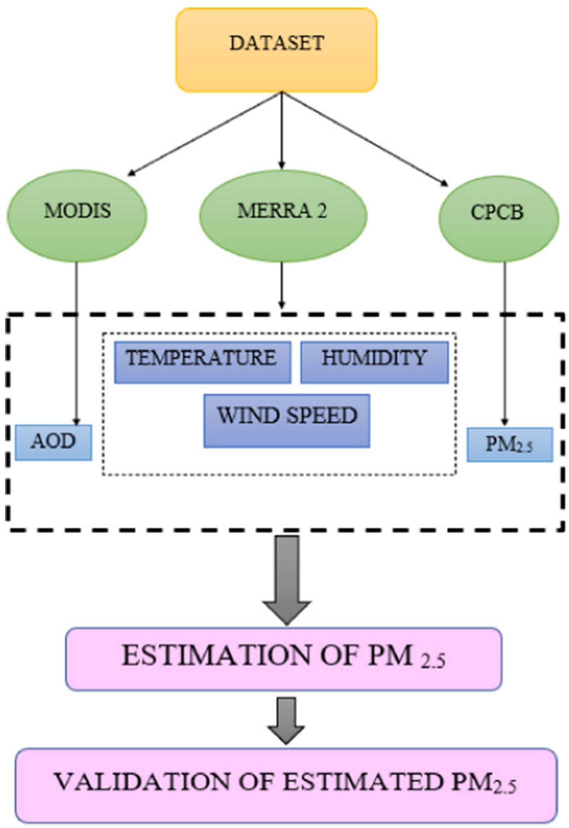

Figure 2
Flowchart depicting the method used to estimate the concentration of $PM_{2.5}$ over Kolkata city

$$PM_{2.5} = a_1 + (b_1 * AOD) \tag{1}$$

here a_1 is the constant derived from the scatter diagram between satellite-retrieved AOD and ground-based $PM_{2.5}$ and b_1 refers to the slope of the intercept line.

3.3.2 Model 2

This model is a multi-linear regression model which considers three additional parameters besides AOD and $PM_{2.5}$ viz. Temperature (T), Relative Humidity (RH), and Wind Speed (WS) at the specified location. In Model 2, the meteorological parameters are the factors that affect $PM_{2.5}$ concentration near the surface of the earth while the AOD features aerosol loading along a vertical column of air.

$$PM_{2.5} = a_2 + (b_{21} * AOD) + (b_{22} * Temperature) + (b_{23} * Relative\ Humidity) + (b_{24} * Windspeed) \tag{2}$$

b_{21}, b_{22}, b_{23}, and b_{24} are estimated regression coefficients derived from scatter plots by plotting each parameter individually with the $PM_{2.5}$ values.

3.3.3 Model 3

$$PM_{2.5} = e^{a_3} + (AOD)^{b_{31}} + (Temperature)^{b_{32}} + (Relative\ Humidity)^{b_{33}} + (Windspeed)^{b_{34}} \tag{3}$$

The equation above (Eq. 3) is an exponential model.

3.3.4 Model 4

$$PM_{2.5} = a_4 + (b_{41} * \ln AOD) + (b_{42} * \ln Temperature) + (b_{43} * \ln Relative\ Humidity) + (b_{44} * \ln Windspeed) \tag{4}$$

The equation above (Eq. 4) is a linear-log model. Through this model, an attempt was made to address the non-linearity in relationship between AOD and

$PM_{2.5}$ assuming that the other factors and parameters follow the power-law function. This model has been employed by previous authors in Agra, India utilizing a logistic regression model instead of a simple multilinear regression model (Chitranshi et al., 2015; Sathe et al., 2019). Improvement was observed in the prediction of PM concentration. Like Model 2, this model also uses three different variables besides AOD. Its logarithmic form is also used which was obtained by log transformation.

In all the above equations (Eqs. 1–4), $a_{1,21,22...}$ are the equation constants and $b_{1,21,22...}$ are regarded as the regression coefficient associated with corresponding variables. The model was fitted on the daily dataset and the output generation, efficiency testing, and estimation were carried out accordingly. Different statistical methods are used to compare and assess model performance. The details of descriptive statistics used can be found in Gupta et al. (2020).

4. Results and Discussion

The annual distribution of $PM_{2.5}$ ground observations and spatial distribution (on a seasonal basis) of MODIS AOD has been discussed. Following this, the $PM_{2.5}$ estimation efforts over the city of Kolkata have been presented. Lastly, the seasonal distribution of the estimated $PM_{2.5}$ has been analysed and discussed utilizing spatial plots.

4.1. Ground-Based $PM_{2.5}$ Observation

Figure 3 represents the daily average concentration of $PM_{2.5}$ for the period of 2019–2021. The highest concentration of $PM_{2.5}$ was observed on January 19, 2021, i.e., 248.46 $\mu g/m^3$, and the lowest was observed on September 2, 2019, i.e., 3.56 $\mu g/m^3$.

The seasonal effects of winter could be the probable reason behind the higher concentration of $PM_{2.5}$ observed during January. One of the dominant effects contributing to higher pollutant concentration is the prevalent lower wind speeds (< 5 m/sec) and localized strong subsidence areas in the winter season (Bangar et al., 2021; Perrino et al., 2011; Rai et al., 2020). Additionally, the pressure changes at different levels hinder the convective movement of an air parcel in turn trapping pollutant ($PM_{2.5}$) concentration near the surface and thus aggravating the pollution levels. Last, northerly to north-westerly winds aid in the transportation of PM generated from the stubble burning events in the States of Northern India towards the States of Bihar, West Bengal (including the city of Kolkata), etc. On the contrary, $PM_{2.5}$ decreased during the month of monsoon predominantly because of the "wash-out" effect of precipitation (Murari et al., 2017).

At last, the overall percentage share of $PM_{2.5}$ concentration groups is depicted in the pie chart (Fig. 3). It is evident that $PM_{2.5}$ concentration ranging from 50 to 100 $\mu g/m^3$ dominated for the entire study period (49.25%) and more than 27% of $PM_{2.5}$ concentration data exceeded the NAAQS daily permissible limit of 60 $\mu g/m^3$. The lowest frequency (0.21%) was observed for $PM_{2.5}$ concentration greater than 200 $\mu g/m^3$.

4.2. MODIS AOD: Spatial Distribution

Figure 4 represents the spatial (seasonal) distribution of MODIS AOD for the study period of 2019–2021. The spatial plots of AOD exhibited strong seasonal variability for each year. It can be observed from Fig. 4, that AOD is significantly high ($\sim$ 0.6–1.2) during the winter season followed by the pre-monsoon season ($\sim$ 0.4–1.0). Further, the AOD values seem to get lowered gradually and decrease sharply during the monsoons ($\sim$ 0.1–0.5).

In Fig. 4, it can be noted the AOD value is lower in 2020 for pre-monsoon and monsoon season, which is the time of complete lockdown implementation. The upsurge in the AOD values can be seen in post-monsoon for the year 2020 after the upliftment of complete lockdown and resuming of industrial activity.

In the year 2019, higher values of AOD can be observed during the winter season (Fig. 4a) throughout the study area. With the arrival of pre-monsoon, the value of AOD starts decreasing gradually (Fig. 4b) and it reaches its lowest level during the monsoon season (Fig. 4c). The washout effect of precipitation resulting in the decrease in AOD value can be observed even in the most polluted part of the city. However, the value of AOD gradually increases

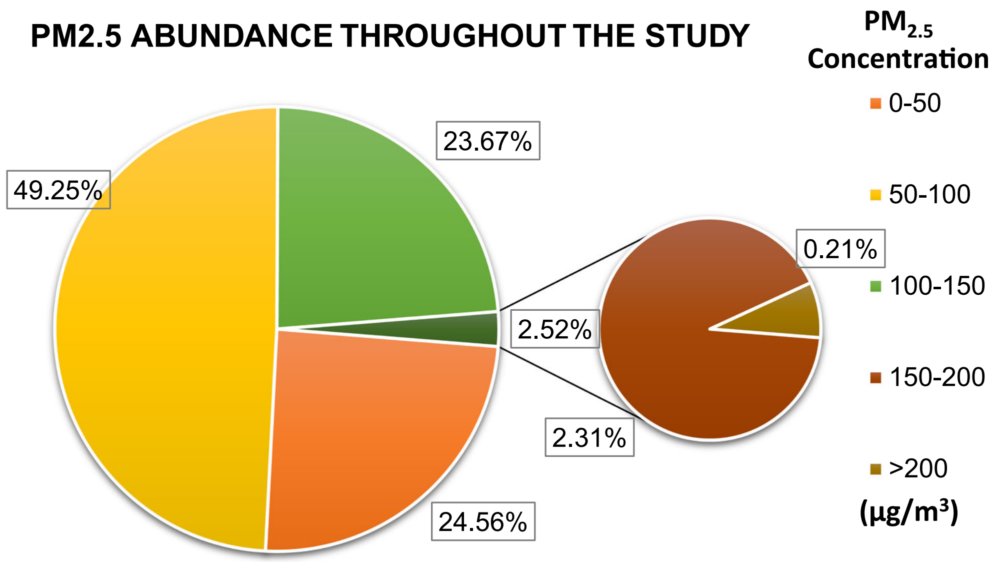

Figure 3
Frequency of daily $PM_{2.5}$ concentration for 2019 to 2021 for the entire study area

in the post-monsoon period (Fig. 4d) in certain patches continuing the general trend. For the year 2020 (Fig. 4e–h) and 2021 (Fig. 4i–l), AOD values followed the same trend with the highest values observed during the winter season and the lowest values observed during the monsoon season.

Pre-monsoon season in India is characterized by strong heating from the sun shining vertically over the Tropic of Cancer. This enhances turbulence and the resultant buoyancy of the air parcel. On the other hand, the winter season is characterized by cool temperatures, and a stable atmosphere hence the low height of the planetary boundary layer favouring the accumulation of particles (Miao et al., 2015). During the pre-monsoon season, the strong heating, low pressure, prevailing winds, and the gradually increasing height of the boundary layer is the cause behind lower values of AOD. During winters, the formation of the inversion layer, stabilization of the atmosphere, and the lower height of the boundary layer prevent any chance of vertical mixing and dispersal. This results in the particles getting accumulated at a certain location which is perceived by the satellite as well as resulting in a comparatively high value of AOD than other seasons. The same trend is seen to be followed throughout the 3-year time of study period.

Strong surface heating during the summers gives rise to an increase in cloud cover followed by large-scale circulation bringing significant oceanic moisture and surface rainfall during the monsoons (Rodwell & Hoskins, 2001). Precipitation during the months of June, July, August, and September enables the wet removal of particles hence reducing particle concentration from the atmosphere. This could be the probable reason behind extremely low AOD values during the monsoon season.

Area-wise variation in AOD values was also analyzed. From Fig. 4, it can be observed that AOD values were the highest for the Bidhannagar region of Kolkata during the winter season of 2019. Apart from this, the value of AOD was either moderate or even low to some extent towards north of the study area. The accuracy assessment of the AOD retrieved from the MODIS satellite has also been performed for its utilization in PM estimation across the Indian subcontinent (Discussed in Sect. 3.1.1).

4.3. *Relationship of Each Parameter with $PM_{2.5}$*

In this section, the association of $PM_{2.5}$ and the meteorological parameter is discussed and in turn, justifies the choice of selecting the parameters as

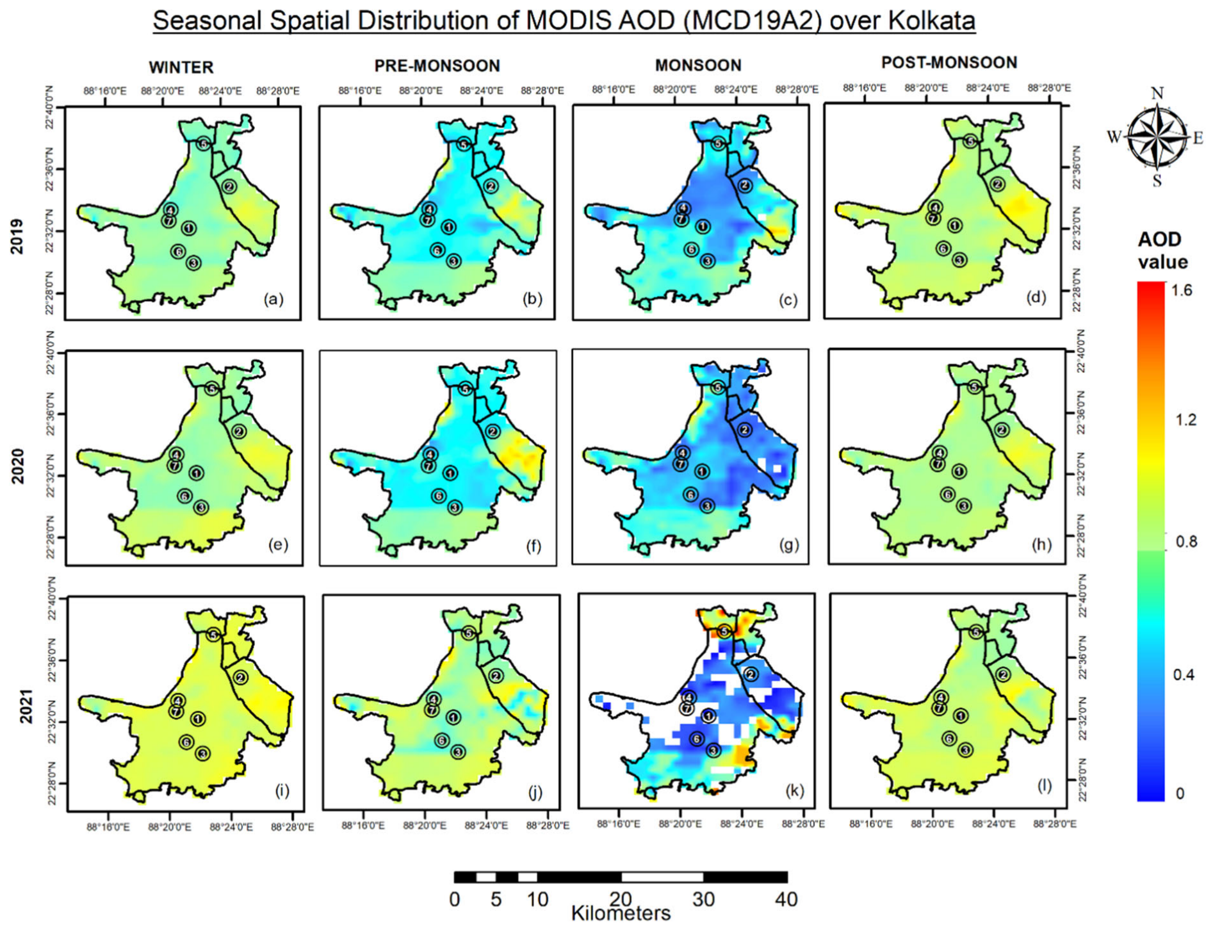

Figure 4

Spatial plot of Seasonal AOD distribution over Kolkata for the years 2019, 2020 and 2021 along with the point locations of CPCB stations (Station ID: 1—Ballygunge; 2—Bidhannagar; 3—Jadhavpur; 4—Fort Williams; 5—Rabindra Bharti University; 6—Rabindra Sarobar; 7—Victoria Memorial)

predictors in estimation models. Temperature could enhance photochemical reactions between particulate precursors (Soni et al., 2018; Tian & Chen, 2010; Wang & Ogawa, 2015). With the increase in temperature, the height of the boundary layer increases allowing more vertical mixing and hence dispersion. As Fig. 5 suggests, the correlation between the temperature and $PM_{2.5}$ was found to be -0.614 which concludes the fact that $PM_{2.5}$ and temperature are negatively correlated. Hence, temperature and concentration of $PM_{2.5}$ are inversely proportional according to this study.

Humidity can directly impact the size of particles considering it promotes hygroscopic growth (Kumar et al., 2011; Soni et al., 2018). The higher the relative humidity, the higher the probability of the formation of particles in quantity which increases the chance of affecting $PM_{2.5}$ concentration. Humidity or more specifically moisture content in the atmosphere provides the raw material needed for the hygroscopic growth of ambient particles. The humidity of a place is weakly correlated with the concentration of PM. The correlation coefficient of the dataset was found to be 0.109 (also depicted in Fig. 5) which proves that although related, the relation between $PM_{2.5}$ and humidity is extremely weak.

Wind on other hand is considered because higher wind speed enables the dispersion of the PM,

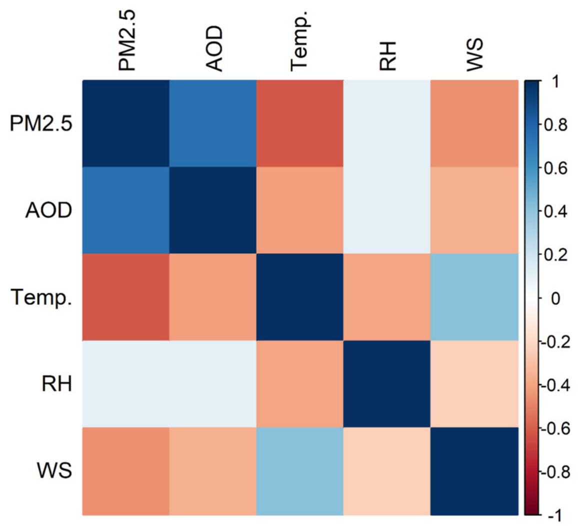

Figure 5
Correlation Matrix of $PM_{2.5}$, AOD, and Meteorological Parameters

lowering the concentration hence the relationship is inversely proportional. From Fig. 5, it is evident that the relationship between $PM_{2.5}$ and Wind speed is moderately negative with a correlation coefficient of − 0.456. The lower the wind, the higher the concentration of particulates observed at any place at a given time.

All the parameters which are mentioned above, directly or indirectly affect AOD values hence PM estimation. Model 2, 3, and 4 takes into consideration every parameter described above. The constants are derived from scatterplots individually and integrated through the model equations to obtain the output.

4.4. Regression Model for $PM_{2.5}$ Estimation

The ground-level $PM_{2.5}$ concentrations, meteorological parameters (Temperature, Relative Humidity, and Wind Speed), and satellite-retrieved AOD integrated at the same spatial and temporal resolutions are used in the present study to develop the regression models. Daily averaged $PM_{2.5}$ concentrations and meteorological parameters are utilized to match the temporal scale of AOD. As the spatial resolution of meteorological data was 0.625° × 0.5°, it is interpolated to 1 km resolution to equal with the spatial resolution of AOD. All the meteorological parameters, AOD, and in-situ measurements of $PM_{2.5}$ used in the study over the region of interest are 24 hourly concentrations and 24 hourly values of $PM_{2.5}$ are estimated.

To check the statistical significance of the model developed for $PM_{2.5}$ estimations, Root Mean Square Error (RMSE), Normalised Mean Bias (NMB), and Mean Absolute Percent Error (MAPE) were calculated along with Correlation (R) for all the models considered in the study. The statistical summary of each model developed is provided in Table 2. Here, the best fit model (MLR) has been emphasized.

The mentioned α-values are intercept, which is a critical component of the regression equation. It represents the value of the dependent variable when all independent variables are equal to zero. While, the mentioned β-values are the slope coefficients. In regression analysis, the slope is a crucial parameter as it represents the change in the dependent variable for a unit change in the independent variable. These coefficients are a statistical measure which is used to quantify the average functional relationship between variables. The slope and intercept both are used to make predictions. Once the regression line is established, it can be used to predict the value of the dependent variable for any given value of the independent variable within the observed range.

Once the PM gets accumulated in the atmosphere due to various sources, their concentrations are strictly modulated by meteorological parameters like Temperature, Relative Humidity, Boundary Layer Height, Wind Speed, Wind Direction, etc. In the present work, the various sources that are responsible for the enhancement of $PM_{2.5}$ were not considered whereas factors that modulate the concentrations in the atmosphere are considered. Moreover, some of the previous studies like Chelani (2019), Chowdhury and Dey (2016), Gupta and Christopher (2009), and Soni et al. (2018) estimated $PM_{2.5}$ concentrations using AOD and meteorological parameters and found satisfactory results. It is evident from the present study that when only AOD and $PM_{2.5}$ (Model 1) are used in the model the R-value is low (0.748) as compared to when meteorological parameters are included. There is a gradual increase in the R-value (0.814) for Model 2 which will be discussed in detail in the later sections. Model 3 and Model 4 however did not produce satisfactory results so are neither used for analysis nor estimation.

Table 2

Descriptive summary of the models developed for the estimation of $PM_{2.5}$ concentration

Model	Model_Type	Parameter_Used	α-Value	β-Value	RMSE (μg/m^3)	Correlation	NMB	MAE	MAPE (%)
1	Simple Linear Regression	$PM_{2.5}$ (Ground Observed); AOD	24.97	$b_1 = 73.771$	37.37	0.748	0.240	29.21	98.86
2	**Multi Linear Regression**	**$PM_{2.5}$ (Ground Observed); AOD; Temp.; RH; WS**	**84.77**	**$b_{21} = +131$, $b_{22} = -4.10$, $b_{23} = +0.31$, $b_{24} = -19.12$**	**22.54**	**0.814**	**− 0.135**	**18.94**	**5.16**
3	Exponential	$PM_{2.5}$ (Ground Observed); AOD; Temp.; RH; WS	103.44	$b_{31} = +1.08$, $b_{32} = -0.07$, $b_{33} = +0.003$, $b_{34} = -0.08$	58.90	0.270	0.723	50.63	197.62
4	Linear-log	$PM_{2.5}$ (Ground Observed); AOD; Temp.; RH; WS	128.40	$b_{41} = +32.56$, $b_{42} = -90.56$, $b_{43} = +0.31$, $b_{44} = -0.01$	467.10	0.295	− 7.761	465.83	1275.00

Model 3 and 4 assume a constant growth rate over time, which may not reflect the actual behavior of PM concentrations. PM levels can be influenced by a wide range of factors, including weather conditions, sources of pollution, and human activities. The above mentioned factors will influence the PM concentration more over a complex terrain such as Kolkata and can lead to nonlinear patterns in PM data which might not be captured by Model 3 and 4 effectively. This could be a probable reason for the poor performance of the models over the region of interest.

Figure 6 depicts the scatter plots between MODIS AOD and $PM_{2.5}$ datasets at Kolkata for the selected period. MODIS AOD (550 nm) data was correlated with $PM_{2.5}$ concentration to assess its applicability to air quality monitoring. MODIS AOD (550 nm) shows promising results (R^2 = 55.87%), and thus in the present study, AOD is considered as one of the model input parameters. Nonetheless, some critical factors are evident to be taken into account to improve the correlation.

4.5. Model Performance

The comparison of estimated $PM_{2.5}$ concentrations against ground observations at the seven stations was utilized for evaluating the effectiveness of developed models in forecasting the $PM_{2.5}$ concentrations over Kolkata (city-level). The correlation between measured and estimated $PM_{2.5}$ through Model 1 (Simple Linear Regression) exhibits a moderate but statistically significant correlation (R = 0.748, RMSE = 37.37 μg/m^3 and MAE = 29.21). The incorporation of meteorological parameters into the model equation (Model 2) aided in improving the $PM_{2.5}$ estimation results when compared with Model 1 results. The $PM_{2.5}$ estimates from MLR model (Model 2) exhibited a positive correlation with the ground-based observations (R = 0.814, RMSE = 22.54 μg/m^3 and MAE = 18.94). For training and calibration of $PM_{2.5}$ estimation models, the study utilizes $PM_{2.5}$ concentrations from seven ground-based monitoring stations maintained by CPCB. After validation of the models, the R-values (0.748) were found to be satisfactory for Model 1. The acquired results provide credit to the accuracy of the developed $PM_{2.5}$ estimation models. It should be

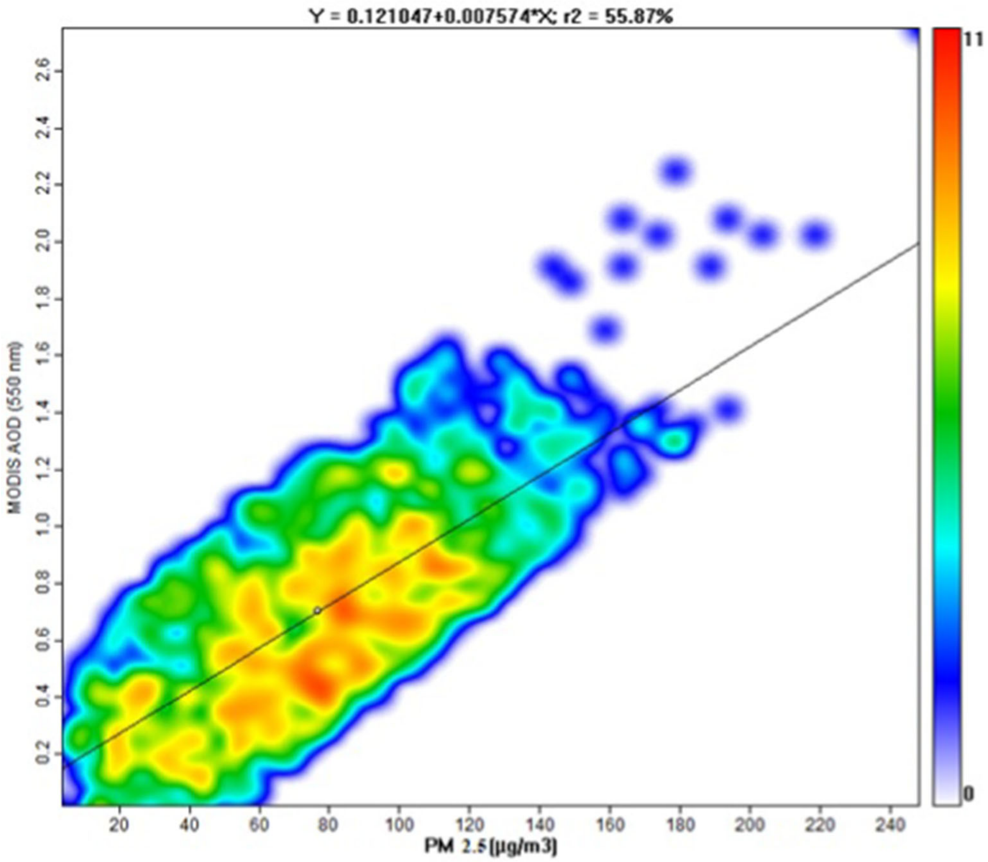

Figure 6
Scatter plot showing correlation coefficient for AOD and $PM_{2.5}$

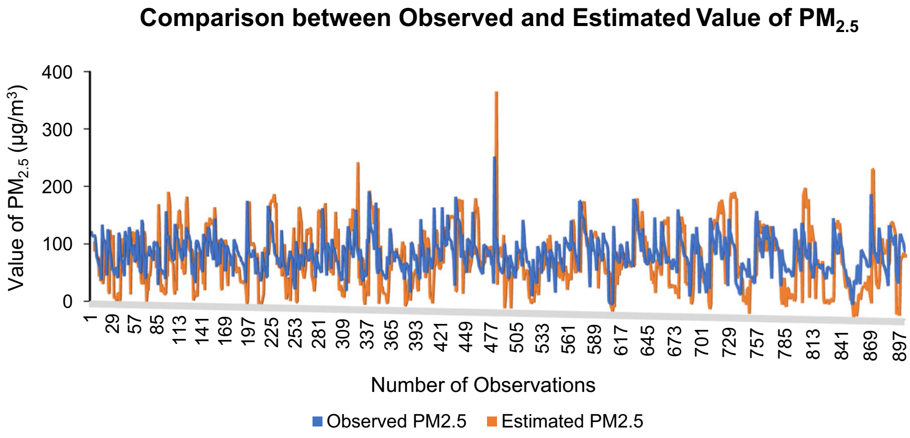

Figure 7
Comparison Graph of $PM_{2.5}$ estimates from Model 2 and Ground-based Observed $PM_{2.5}$ concentration

noted that among all the models, $PM_{2.5}$ estimates obtained from Model 2 were found to be well-correlated with ground observations with an R-value of 0.814. This indicates that the estimated values are very close to the ground observations hence the model performance can be categorized as good. Model 3 and Model 4 however did not produce satisfactory results so are neither used for analysis nor estimation.

Figure 7 shows the daily profile of $PM_{2.5}$ concentrations during the test period for observed and modeled values (obtained from Model 2). The pattern of $PM_{2.5}$ concentrations is well captured by the model representing both peak and dip values. However, the model tends to underestimate the concentration values consistently. This provides an opportunity for improvement of the model equation developed for city-scale estimation.

Additionally, the station-wise $PM_{2.5}$ concentrations have been analyzed on a seasonal basis using model estimates (Fig. 8). The value of $PM_{2.5}$ as depicted in Fig. 8 is highest during winter and post-monsoon seasons. Station-wise data revealed that during the winter season the highest concentration of $PM_{2.5}$ was observed for Jadhavpur in 2019 (34.7 μg/m^3) Ballygunge in 2020 (93.47 μg/m^3) and Victoria Memorial in 2021 (96.67 μg/m^3). In the pre-monsoon season, the highest values were recorded at Ballygunge throughout 2019 to 2020 and even for the monsoon of 2019. In the post-monsoon season, Ballygunge station always had the highest values. In the future step, the developed model will be applied to other Indian cities, and the incorporation of more parameters into the model equation will be considered as predictors for more detailed and accurate estimation.

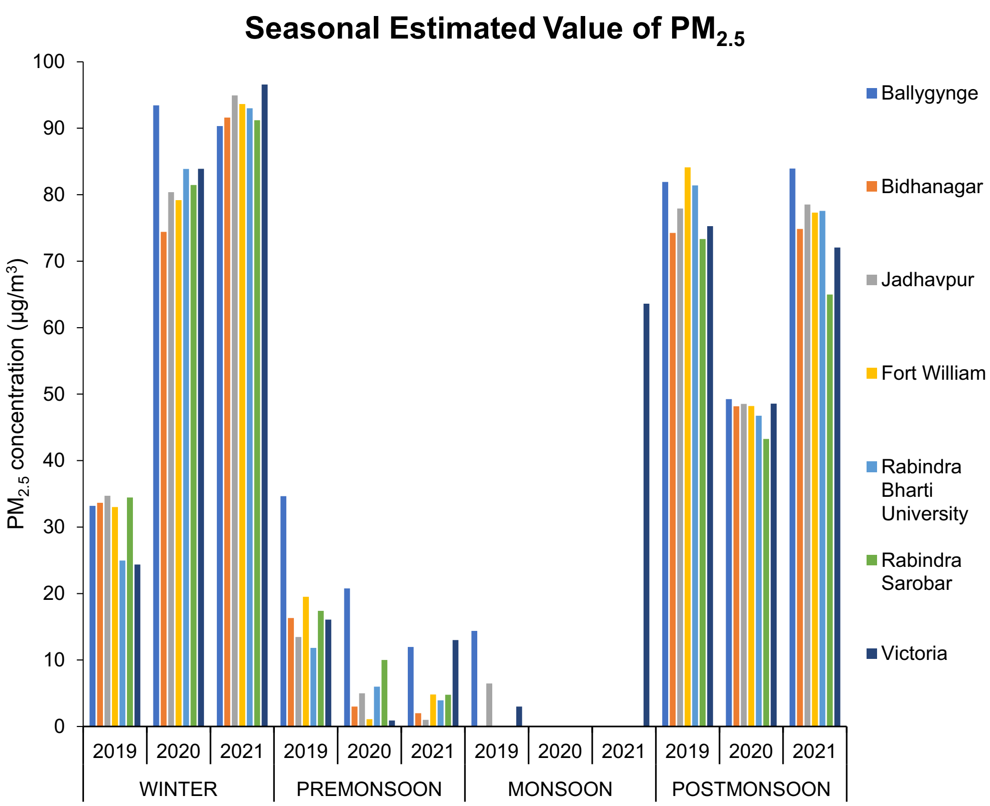

Figure 8
Graph depicting the seasonal estimated value of $PM_{2.5}$ for the year 2019–2021

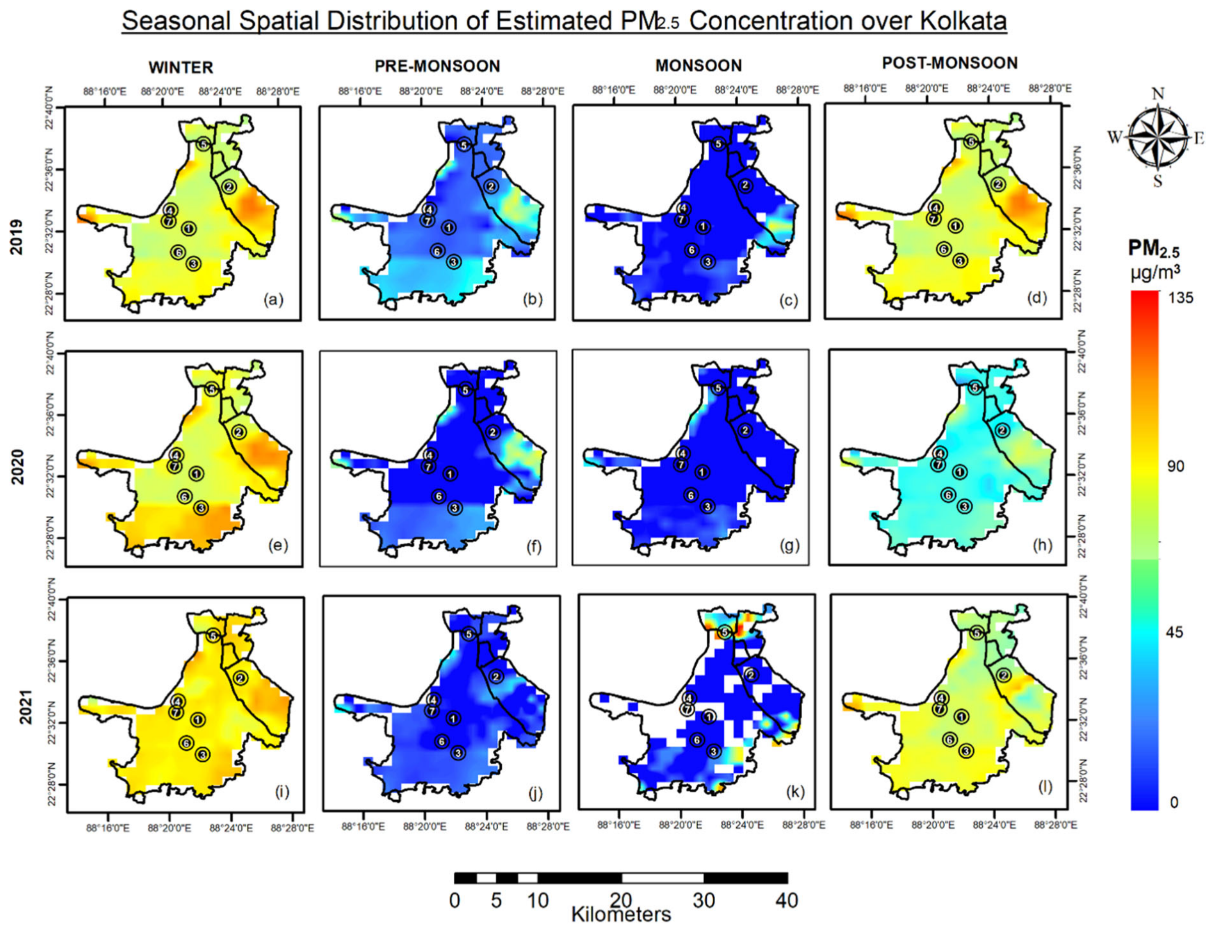

Figure 9
Seasonal Spatial plot of $PM_{2.5}$ concentration over Kolkata for the years 2019, 2020 and 2021 along with the point locations of CPCB stations (Station ID: 1—Ballygunge; 2—Bidhannagar; 3—Jadhavpur; 4—Fort Williams; 5—Rabindra Bharti University; 6—Rabindra Sarobar; 7—Victoria Memorial)

4.6. *Estimated $PM_{2.5}$: Spatial Distribution*

The seasonal-mean spatial distribution of the estimated $PM_{2.5}$ concentrations over the entire Kolkata from 2019 to 2021 are shown in Fig. 9 at 1×1 km spatial resolution, using the MLR model (Model 2). The seasonal-mean spatial mapping was performed using QGIS software.

The trend that is followed by AOD is the same as exhibited by the estimated $PM_{2.5}$, observed from the seasonal spatial plots (Fig. 4). The cases of high $PM_{2.5}$ concentrations are restricted to the adjoining district of Bidhannagar. Central Kolkata seems to have a low concentration of $PM_{2.5}$ which can be attributed to the fact that the region has dense vegetation cover and some parts of the area is under military control hence every kind of activity is restricted.

The Bidhannagar area which shows high $PM_{2.5}$ concentrations is the developed corner of the city and the very same location houses the dumping ground for the municipal solid waste of the city. The waste management process involves burning garbage which can be one of the possible reasons for the high pollution apart from vehicular emissions from one of the busiest traffic regions in the city.

On average, the maximum value of the estimated $PM_{2.5}$ concentration has reached up to 120 μg/m^3. According to NAAQS, for residential areas, the maximum permissible limit of $PM_{2.5}$ is 60 μg/m^3, and on basis of this standard, it can be inferred that the air quality of Kolkata is more or less good except for some areas where the pollution level is extremely high and fulfills the standards set up by NAAQS.

In addition, from the seasonal analysis, it is observed that the mean concentration of $PM_{2.5}$ over the entire city of Kolkata was high during the winter season and the concentration level decreases gradually with the approach of the pre-monsoon and decreases sharply during the monsoon season but starts to increase gradually again from the post-monsoon season.

5. Conclusions

From the above study, it can be inferred that $PM_{2.5}$ and AOD values vary significantly through different seasons with values peaking up during the winter season and dipping during the monsoon season. From the process followed, it can be further concluded that out of the four different models used, Model 2 was the best fit model. The correlation coefficient between the ground-based and the estimated $PM_{2.5}$ values was found to be 0.814 for Model 2. The normalized mean bias (NMB) value was − 0.135, the mean absolute error (MAE) was 18.94, and the mean absolute percent error (MAPE) was 5.16%. The estimated $PM_{2.5}$ values were able to capture changes in $PM_{2.5}$ concentration on the ground and the same was proved by the results derived.

The developed model (Model 2) thus can be used for future research work involving $PM_{2.5}$ concentration over areas where ground-based observation sites are not always present. This study will aid different governmental authorities and public health agencies to frame various programs and policies concerning public health about the negative effects of particulate pollution on human health.

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Author Contributions All authors contributed to the study's conception and design. Material preparation, data collection and analysis were performed by JS and SS. The first draft of the manuscript was written by SS and conceptualized by SP. The work was Initiated by SV. SS collected the aerosol data and formatted with the help of JS. SS and JS has plotted and started the analysis with the mentorship of Sunita and Swagata. MM curated the data and supervised the work at different stages. All authors commented on previous versions of the manuscript. All authors read and approved the final manuscript.

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Declarations

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