Real-time PM 2.5 forecast over Delhi: Performance of high resolution (400 m) WRF-Chem model integrated with data assimilation and dynamical downscaling

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Abstract

We present a very high-resolution (400 m) operational air quality forecasting system developed to alert citizens of Delhi and the National Capital Region (NCR) about acute air pollution episodes. Such a high-resolution system has been developed for the first time and is evaluated during October 2019-February 2020. The system assimilates near real time aerosol observations from in situ and space-borne observations in the WRF-Chem model to produce a 72-h forecast every day in a dynamical downscaling framework. The assimilation of aerosol optical depth and surface PM 2.5 observations improves the initial condition for surface PM 2.5 by about 45 µg/m 3 (about 50%). The accuracy of the forecast degrades slightly with time as mean bias increases from +2.5 µg/m 3 on the first day to-17 µg/m 3 on the third day of forecast. Our forecasts are found to be very capable both for PM 2.5 concentration and unhealthy/ very unhealthy air quality indices categories. 2

Real-time $PM_{2.5}$ forecast over Delhi: Performance of high resolution (400 m) WRF-Chem model integrated with data assimilation and dynamical downscaling

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Abstract

We present a very high-resolution (400 m) operational air quality forecasting system developed to alert citizens of Delhi and the National Capital Region (NCR) about acute air pollution episodes. Such a high-resolution system has been developed for the first time and is evaluated during October 2019-February 2020. The system assimilates near real time aerosol observations from in situ and space-borne observations in the WRF-Chem model to produce a 72-h forecast every day in a dynamical downscaling framework. The assimilation of aerosol optical depth and surface $PM_{2.5}$ observations improves the initial condition for surface $PM_{2.5}$ by about 45 μg/m^3 (about 50%). The accuracy of the forecast degrades slightly with time as mean bias increases from +2.5 μg/m^3 on the first day to -17 μg/m^3 on the third day of forecast. Our forecasts are found to be very capable both for $PM_{2.5}$ concentration and unhealthy/ very unhealthy air quality indices categories.

1. Introduction

Being the second most populated megacity in the world, Delhi faces enormous challenges due to a range of issues including adverse air pollution episodes during the winter season (Ghude et al., 2008; Beig et al., 2019; Chandra et al., 2018; Hakkim et al., 2019; Takigawa et al., 2020), which pose a higher health risk as a result of substantial population density exposure (Beig et al., 2013; Chate et al., 2013; Ghude et al., 2016; Guttikunda and Goel, 2013; Spears et al., 2019). In recent years, particulate matter of aerodynamic diameter smaller than 2.5 µm($PM_{2.5}$) has dominated severe air pollution episodes frequently observed during the winter season, affecting daily life in Delhi (Chowdhury et al., 2019; Jethva et al., 2019). Thus, managing air quality with practical mitigation options has emerged as a complicated task without compromising the intended growth in the overall infrastructure development, industries, and service sectors.

The Government of India(GOI) is committed to enforce policy-driven measures to reduce the pollutant emissions. The National Clean Air Program(NCAP) initiated by the GOI targets significant reduction of surface $PM_{2.5}$ concentration by the year 2024. A Graded Response Action Plan(GRAP) has been designed for the National Capital Region(NCR) that allows pollution control authorities to reduce the magnitude of predicted air pollution for different air quality indices(AQI) categories. Activation of different GRAP measures requires information of forthcoming extreme air pollution episodes so that effective temporary control measures can be identified early and implemented in advance. Therefore, GOI mandate required the Ministry of Earth Science(MoES) to develop an operational high-resolution modelling for the NCR region. In response to the mandate, MoES institutions, Indian Institute of Tropical Meteorology(IITM) and India Meteorology Department(IMD), has developed a first very high-resolution (400 m) chemical weather forecasting capability in mutual collaboration with U.S. National Centre for Atmospheric Research(NCAR). The initial capability was developed for Delhi during 2018 based on weather research and forecasting model coupled with online chemistry module(WRF-Chem) at horizontal resolution of 2 km (Ghude et al., 2020). The first version of the forecasting system has been found to significantly improve air quality decision-making activity by reducing biases in 72-h $PM_{2.5}$ forecasts to a greater extent (Kumar et al., 2020). However, that system struggled to predict the absolute $PM_{2.5}$ levels during very acute air pollution episodes characterized by surface $PM_{2.5}$ mass concentrations greater than 350 $\mu g/m^3$ (Ghude et al., 2020).

To further enhance the air quality decision-making activity the modelling framework was further extended to produce forecast fields of $PM_{2.5}$ concentrations at much higher resolution of 400 meters. To the best of our knowledge, none of the operational centres are currently providing short-term operational air quality forecasts at a spatial scale of 400 x 400 m^2 covering approximately 50 km^2 areas. This is the first attempt to develop and evaluate the performance of $PM_{2.5}$ forecast in a highly polluted environment using integration of dynamical models with chemical data assimilation. This high-resolution forecasting system consists of a newly developed high-resolution (400 m) emission inventory for Delhi, assimilation of satellite aerosol optical depth(AOD) and surface $PM_{2.5}$ concentrations from a dense air quality monitoring network in Delhi to constrain the regional and local background of aerosols, and ingests near real-time fire emissions, and applies high-resolution dynamical downscaling into the WRF-Chem. $PM_{2.5}$ forecasts at 400 m resolution were made operational in October 2019.

Here, we provide a brief description of the operational high-resolution forecasting system, highlight the impact of data assimilation, and evaluate the quality of the $PM_{2.5}$ operational forecast for the latest winter season in Delhi. We show that the forecast falls within the expected uncertainties and, therefore is suitable for operational air quality early warning for the Delhi region.

2. Air quality forecasting system

The complete overview of the air quality early warning system is given in the schematic shown in Figure S1. The major components of the system are a) high-resolution numerical predication model WRF-Chem, b) gridpoint statistical interpolation (GSI) based three-dimensional variational(3D-var) data assimilation integrated with dynamical downscaling, c) observational data and emission pre-processer, d) post analysis, and e) public dissemination system(https://ews.tropmet.res.in/). The system operates overnight and disseminates the information in the morning for the next 72 hours.

2.1 Modelling setup

The core of the forecasting system consists of the regional WRF-Chem Version 3.9.1 configured in a three domain set-up with the outer domain covering northern part of the Indian subcontinent at a horizontal resolution of 10 km, the second domain covering the NCR and neighboring state at 2 km resolution, and the innermost domain covering Delhi at 400 m resolution (Figures S1 and S2). The meteorological initial and boundary conditions are based on the analysis and forecast product (Ensemble-Kalman filtering) produced by the IITM-Global Forecasting System (IITM-GFS, T1534) spectral model at 12.5 km grid resolution available at every three hours. The outer domain (D1) is provided with the six-hourly chemical boundary conditions from the MOZART-4 10-year climatology. However, chemistry output from the D1 domain every three-hour interval was dynamically used to establish a chemical boundary for the WRF-Chem inner domain (D2). Similarly, the output from the D2 domain was dynamically used to establish boundary conditions for the final 400 m domain (D3). Physical and chemical parameterizations used in the model are listed in Supplementary Table ST1. The forecast was run with MOZART-4 gas-phase chemistry linked to GOCART aerosol scheme(MOZCART). In the GOCART, aerosol nitrates and secondary organic aerosols are missing and are a source of uncertainty in the estimated $PM_{2.5}$. However, this scheme is computationally most efficient than the other advanced aerosol schemes (e.g., MOZAIC), and therefore it is suitable for the operational forecast.

2.2 Satellite AOD and Surface $PM_{2.5}$ data assimilation

We used three-dimensional variational method(3D-Var) component of the community Gridpoint Statistical Interpolation(GSI) system Version 3.5. The 3D-var scheme blends the information from the satellite AOD and surface $PM_{2.5}$ observations, and iteratively minimizes a cost function J that depends on observation and background error covariance matrices as defined in equation (1).

$$\mathrm{J}(\mathbf{x}) = \frac{1}{2}(\mathbf{x} - \mathbf{x_b})^{\mathrm{T}}\mathbf{B}^{-1}(\mathbf{x} - \mathbf{x_b}) + \frac{1}{2}(\mathrm{H}(\mathbf{x}) - \mathbf{y})^{\mathrm{T}}\mathbf{R}^{-1}(\mathrm{H}(\mathbf{x}) - \mathbf{y}) \quad (1)$$

where $\mathbf{x}$ represents the state vector required in AOD calculation, $\mathbf{x_b}$ represents the "a priori" information about $\mathbf{x}$ and is referred to as background, $\mathbf{B}$ is the background error covariance (BEC) matrix, H is the forward operator that transforms WRF-Chem aerosol chemical composition to AOD following Liu et al. (2011), $\mathbf{y}$ represents the MODIS AOD retrievals, and $\boldsymbol{R}$ is the observation error covariance matrix. BEC statistical parameters are calculated using two 24-h WRF-Chem forecast initialized at 00 z with different meteorological, anthropogenic emissions and biomass burning emissions to account for the uncertainties in both meteorology, anthropogenic, and biomass burning emissions (Kumar et al., 2019).

Observations from MODIS overpasses at 10:30 and 1:30 L.T. at 10 km resolutions and hourly mean surface $PM_{2.5}$ observations from the 37 monitoring stations (Figure S3) across Delhi are collected at the analysis time on 0900 UTC assimilation cycle. GOCART has sixteen aerosol species, and all are adjusted directly by AOD and surface $PM_{2.5}$ assimilation. More details on the AOD assimilation for the GOCART scheme can be found elsewhere (Ghude et al., 2020; Kumar et al., 2020). Every day, the chemical fields are initialized from the previous WRF-Chem forecast at 0900 UTC, aerosol initialization is updated through assimilation, and meteorology is refreshed using the IITM-GFS forecast. To understand how much the assimilation of surface $PM_{2.5}$ and satellite AOD observations changes the WRF-Chem $PM_{2.5}$ at the initialization time on every day towards the observed reality, averaged surface $PM_{2.5}$ simulated by the model before and after assimilation are compared with the observations at 0900 UTC assimilation cycle (Figure 1). Before assimilation, the simulated $PM_{2.5}$ at the initialization time significantly underestimates the observed $PM_{2.5,}$ and assimilation pushes WRF-Chem initial condition very close to the observations. The average observed $PM_{2.5}$ is about 133±88 μg/m^3, whereas simulated $PM_{2.5}$ before assimilation and after assimilation is estimated as 90±36 μg/m^3 (mean bias = -32%) and 135±83 μg/m^3 (mean bias = +1%), respectively. This indicates that assimilation on an average improves the initial condition for $PM_{2.5}$ by ~45 μg/m^3 (about 50%) at the assimilation cycle.

3.3. Emissions and observations

Two anthropogenic emission databases are included in the forecasting setup. We used 2010 EDGAR-HTAP emissions at 10 km resolution for the outer (D1) and intermediate (D2) domains and scaled to 2019 using scaling factors given in Venkataraman et al. (2018). This data was used only for the area outside the Delhi region. For Delhi itself (D3), we used 400 m resolution emission inventory for the year 2018 developed under the MoES(Figure S4)

System of Air Quality and Weather Forecasting and Research(SAFAR) project. For the outer and intermediate domain, the original 400 m emissions were processed using a mass-conserving approach to match the 10 km and 2 km grid spacing so that the total mass emitted is the same before and after re-grinding. We adopted diurnal variation in emissions from a recent study by Govardhan et al. (2019). We performed emission sensitivity simulations by keeping EDGAR emissions for the entire model domain and then replacing the Delhi region with high-resolution Delhi emission inventory. We find that $PM_{2.5}$ mass concentration simulated by the EDGAR largely under-predict (bias = -52%) the observed $PM_{2.5}$ mass concentrations in Delhi, whereas as high-resolution inventory over-predict by 36% during the winter season (Figure S5). Additional simulation where emissions are reduced by 40% shows better agreement with observations (bias =3%). Therefore, in the forecasting setup, we choose emissions reduced by 40% over the Delhi region.

Model of Emissions of Gases and Aerosols from Nature (MEGAN; Guenther, 2007) is used to include interactive biogenic emissions. Dust emissions are based on the online AER/AFWA scheme (Jones and Creighton, 2011). Our recent study shows that post-monsoon biomass burning emission significantly affects the air quality in Delhi (Kulkarni et al., 2020). Therefore, an accurate representation of fire emissions is essential for the quality of the forecast. Most of the near real-time biomass burning emission estimate is available with a time lag of one day and thus operational air quality forecasts are forced to assume persistent fire emissions over the forecast cycle. Here, we have developed a pre-processor based on the high-resolution Fire INventory from NCAR (FINN, Wiedinmyer et al., 2011) to derive fire emissions for the forecast day instead of using the estimates from a previous day. We first developed a historical daily gridded (at the model grid spacing) data set of biomass burning emissions from 2010 to 2018. Secondly, daily fire location information is obtained from the near real-time MODIS-C6 active fire data from FIRMS (https://firms.modaps.eosdis.nasa.gov/). Finally, the historical fire emissions are used to represent fire emissions in all the model grids showing the fire activity. To include the fire emissions for the next two days, we calculated the historical fire frequency for each day and for each model grid based on a 10-year gridded data set. We include the fire emissions only in those grid cells where frequency of fire count is more than 50%.

The $PM_{2.5}$ data set used in the study are obtained in near real-time from the 37 air quality monitoring stations operated by the Central Pollution Control Board(CPCB), Delhi Pollution Control Committee(DPCC), and IITM. The instruments are calibrated, and the measurements are quality controlled (https://cpcb.nic.in/quality-assurance-quality-control/). In addition to the CPCB quality control, we apply additional filters to remove single spikes, $PM_{2.5}$ measurements above 1500 μg/m^3, observations from the period corresponding to instrument malfunction (Kumar et al. 2020). The details of these monitoring locations are given in Table ST2 in the supplement, and the geographical locations are shown in Figure S3. Statistical evaluation metrics such as mean bias(MB), Pearson's correlation coefficient(r), normalized mean bias(NMB), normalized mean fractional error(NME) (Yu et al., 2006; Zhang et al., 2006) are used to evaluate the performance of $PM_{2.5}$ forecasts.

3. Result

3.1 Performance of the $PM_{2.5}$ forecast

The air quality forecast verification period (21 October 2019–02 February 2020) selected here for Delhi was dominated by the large-scale open biomass burning in October and November followed by wintertime stable meteorological conditions conducive for build-up of

$PM_{2.5}$ pollution in Delhi. An example of the spatial distribution of average $PM_{2.5}$ concentration from day 1 forecast is shown in Figure 2a. As expected, the 400 m domain resolves emission sources in Delhi much better than the 10 km and 2 km domains (Figure S6). At finer grid resolution, $PM_{2.5}$ hotspots associated with the industrial, dense residential, major traffic junctions, and high-density vehicular traffic roads can be clearly distinguished from Figure 2a. Daily forecast (Figure 2b) tracts the daily variation of mean observations quite well in the NCR region. However, model performance for the $PM_{2.5}$ forecast for individual monitoring stations (supplementary table ST2) generally shows that the NMB varies from -46% to 85% among the 37 stations located across the NCR region. Out of 37 stations, 24 individual stations (65% of stations) show NMB within ±30%, and 5 stations (13% of stations) show NMB more than 50%.

To more closely examine the model performance for the $PM_{2.5}$ forecast specific to the NCR, we compared the hourly time series of mean $PM_{2.5}$ forecast with observations. The NCR region contains 37 monitoring stations, and model forecasts from the locations of all these monitoring stations are extracted and average to get $PM_{2.5}$ time series for Delhi. The comparison for the first, second, and third day of forecast at 400 m resolution domain is depicted in Figure 3. The forecast captures the temporal variability in $PM_{2.5}$ observation quite well on most of the days. On two occasions, 2–4 November and 12–16 November, the model largely failed to capture extremely high $PM_{2.5}$ values observed in the NCR region. However, very-poor pollution events occurred on 20–22 November, and very-poor to sever air quality events on 5–12 December, 19–22 December, 19–21 December, 29 December 2019–5 January 2020 were captured very well by the forecast. The sudden drop in $PM_{2.5}$ levels (e.g., on 14 December, 7 January, 24 January, etc.) followed by the very-poor to sever events were also captured very well by the model. The temporal variation in observed $PM_{2.5}$ over Delhi and pollution episodes are driven mainly by the frequent large scale open biomass burning and wintertime synoptic-scale meteorological condition in combination with the large anthropogenic emissions in this region. Figure 3 shows that the model has a very good ability to capture this variability and indicates that the forecast system is very capable of issuing $PM_{2.5}$ forecasts associated with urban pollution and synoptic-scale meteorological events.

The performance statistics for hourly mean $PM_{2.5}$ forecast for the first, second and third day is evaluated by examining MB, RMSE, r, NMFB, and NMFE (Table 1). Following Morris et al. (2005), we have adopted three levels of performance criteria for fractional bias and error to evaluate the forecast performance (supplementary table ST3). It can be seen that the magnitude of MB on the first day of hourly forecast was quite low (2.5 $\mu g/m^3$), and slightly under predicted by about -9 $\mu g/m^3$ and -17 $\mu g/m^3$ on the second and third day of the forecast, respectively. Table 1 reveals that $PM_{2.5}$ forecast performed close to excellent criteria on day 1 since the NMFB and NMFE were within 1.3% and 36.3%, respectively. The model performance was quite good on day 2 and day 3 with fairly low NMFB (<±10%), and NMFE was within ±40%. Performance statistics on daily mean $PM_{2.5}$ time series show fairly excellent performance on all the three days of forecast since NMFB and NMFE were within ±10% and 29%, respectively. The correlation coefficient (r) is around 0.5 for the hourly forecast and 0.6 for the daily mean forecast. It appears from Figure S7 that there is a considerable scatter between observed and predicted $PM_{2.5}$. Forecasts generally show a tendency to under predict the higher values and slightly over predict the lower values, consistent with the other studies (Eder et al., 2006, 2010). Efforts are underway to investigate why this underestimation in higher values occurs and whether it is the result of errors in the meteorological, boundary condition, emission, or chemical factors.

3.2 Performance of the Air Quality Index (AQI) forecast

The main interest in the application of high-resolution forecast is to provide timely air quality alerts to the public in the NCR region, particularly for the Poor to Severe AQI category. As per the CPCB guidelines, AQI category is classified as poor for AQI range 201-300, very-poor for AQI range 301-400, and severe for AQI range 401 and above. Therefore, it is essential to evaluate the applicability of the system to simulate the correct AQI values, as these are typically disseminated to the general public rather than the actual $PM_{2.5}$ mass concentrations. Accordingly, hourly AQI values for $PM_{2.5}$ based on 24-h $PM_{2.5}$ standard was calculated based on National Ambient Air Quality Standard(NAAQS), and break-point concentration suggested in the CPCB notification (see supplementary Table ST4). It can be seen in Table 1 that the magnitude of MB for overall AQI values (0–500) was slightly higher (about 22 units) on the first day of forecast compared to MB observed on the second day (10 unit) and third day (<1 unit). However, following the Morris et al., (2005) criteria, the AQI forecast on all three days performed excellently, since NMFB and NMFE were within ±6% and 18%, respectively. The statistical performance (Supplementary Table ST5) indicates that the forecast over-predicts poor air quality category by about 22% on day one and by about 19% and 16% on days two and three, respectively. AQI forecast on all three days in poor category performed fairly good since NMFB and NMFE were within ±22% and 22%, respectively. For a very-poor category, the AQI forecast performed excellent on all three days (NMFB <5% and NMFE <9%) of the forecast. In comparison, statistics show that forecast under-predicts the severe category by about 14% on day one and by about 17% and 21% on day two and day three, respectively. On the first day, the AQI forecast for the severe category performed excellently (NMFB <14% and NMFE <17%), while it performed reasonably well on day two and day three (NMFB <21% and NMFE <21%). Overall, the forecast falls within the expected uncertainties and, therefore, is suitable for operational air quality forecast for the Delhi region.

3.3 Skill score for categorical AQI forecast

To assess the skill of real-time forecast, that is, whether the forecast will fall in unhealthy (AQI >201), or very-unhealthy (AQI >301) or critical category (AQI >401), false alarm rate(FAR), probability of detection(POD) or hit rate, critical success index(CIS) and accuracy, was calculated according to Kang et al. (2005) and Eder et al. (2010). Supplementary table ST6 describes the equations that are used to calculate the skill score of the categorical AQI forecast. Table 1 presents the skill score for the unhealthy, very-unhealthy, and critical category of AQI for winter season. The forecast accuracy for unhealthy category (i.e., forecast that correctly predicted the unhealthy or no-unhealthy AQI) showed the accuracy values to be >88% on all the three days. The skill score for the POD and CSI is relatively promising with a value grater that ~0.9, which indicates that the model has reasonable good predictive accuracy in predicting the unhealthy air quality conditions with respect to a total number of the observed air quality hours. Also note that FAR is quite low (~10%) for the unhealthy category, which indicates that the performance of the real-time high-resolution forecast was excellent for both unhealthy category and non-unhealthy category of air quality. For the very-unhealthy category, although the skill score of POD (>0.9) is excellent, compared to the unhealthy category, the skill score for the CSI is a little low (~0.7), and FAR is a little high (20-30%) on all three days of forecast. However, the skill score overall indicates excellent performance for predicting air quality in the very-unhealthy category. On the other hand, the skill score shows moderate performance for the severe category of events on all three days. Table 1 indicates that compared to the unhealthy and very-unhealthy category, the skill score for POD and CSI is low (<0.35) on day one and day two of forecast and further declines on day three. Note that the accuracy of the forecast is about 80%, and the skill score for FAR does not show a significant increase compared to the other two categories, which indicates the moderate ability of the forecasting system to predict the extremely high pollution events in NCR region correctly. Some of the causes of unsuccessful prediction of accurate extremely high pollution events may include difficulties in simulating processes like boundary layer height, synoptic advection, and synoptic-scale conditions and choice of aerosol module. Our future studies will investigate the role of these processes in predicting the extreme $PM_{2.5}$ pollution events in the NCR region.

4. Conclusion

This study aims to demonstrate the efficacy of a prototype very high-resolution operational air quality forecasting system developed to issue timely warning to the citizens of Delhi about forthcoming air pollution episodes. The system is based on the WRF-Chem model integrated with satellite AOD and surface $PM_{2.5}$ data assimilation and dynamical downscaling. Performance of the system was evaluated both for $PM_{2.5}$ mass concentration and AQI categories to assist both local forecaster and air quality model developers. Both AOD and surface $PM_{2.5}$ data assimilation, on an average, improves the initial condition for $PM_{2.5}$ by about by ~45 µg/m^3 (about 50%) at the assimilation cycle. Model evaluation shows that finer-resolution $PM_{2.5}$ forecasting system is capable of issuing reliable forecasts for Delhi during winter season both for $PM_{2.5}$ concentration and AQI in particular for unhealthy and very-unhealthy AQI categories, within the expected uncertainties. On the other hand, verification statistics with reference to severe categories show moderate skill and may require further improvement in the forecast. Although finer-resolution $PM_{2.5}$ forecast captures the spatial variability in emissions, it is desirable to have an accurate forecast at every individual station with a high-resolution forecast. The model showed moderate performance to capture the accurate spatial concentration across the NCR region and requires further improvement. We recognize that the accuracy of the high-resolution emission inventory, choice of aerosol model, chemical mechanism, and boundary layer parameterization will continue to be a challenge to forecast the $PM_{2.5}$ at individual point monitoring locations in a highly polluted environment. Efforts are underway to explore the sensitivity of these parameters to the accuracy of location-specific $PM_{2.5}$ forecast. For the first time, the system was also used by the environmental pollution control authorities to make the decision on imposing/lifting the restriction on construction activities and regulating the heavy vehicle inflow in Delhi region during the pollution/no-pollution events. This has significantly contributed to the build-up the trust to the end-users and policy-makers for taking science-based well-informed decisions and actions for important public services in India.

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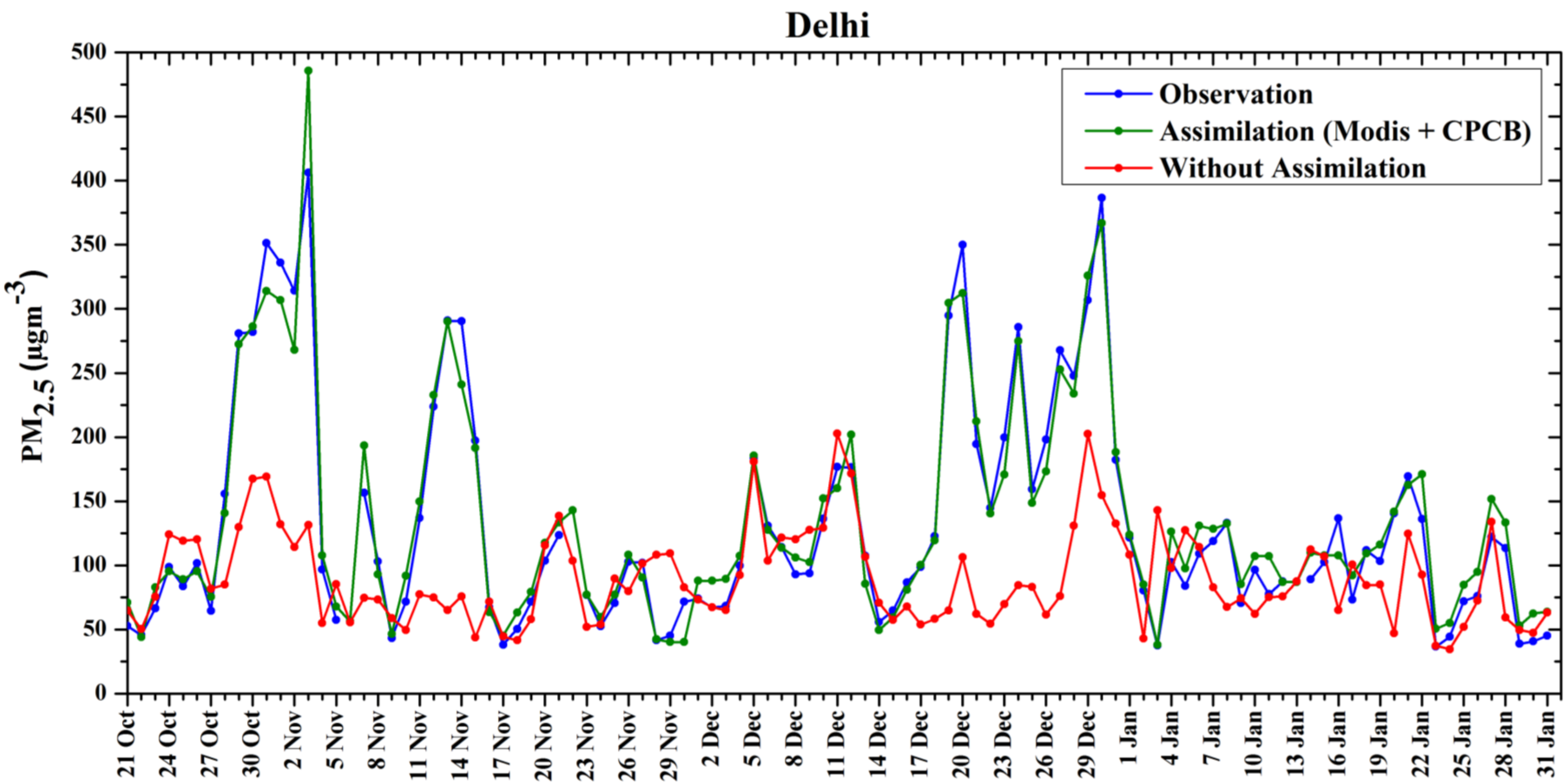

Figure 1: Averaged surface $PM_{2.5}$ simulated by the model before (red) and after (green) assimilation at 0900 UTC assimilation cycle (Figure 1) and its comparison with observed mean $PM_{2.5}$ over Delhi during 21 October 2019 to 01 February 2020.

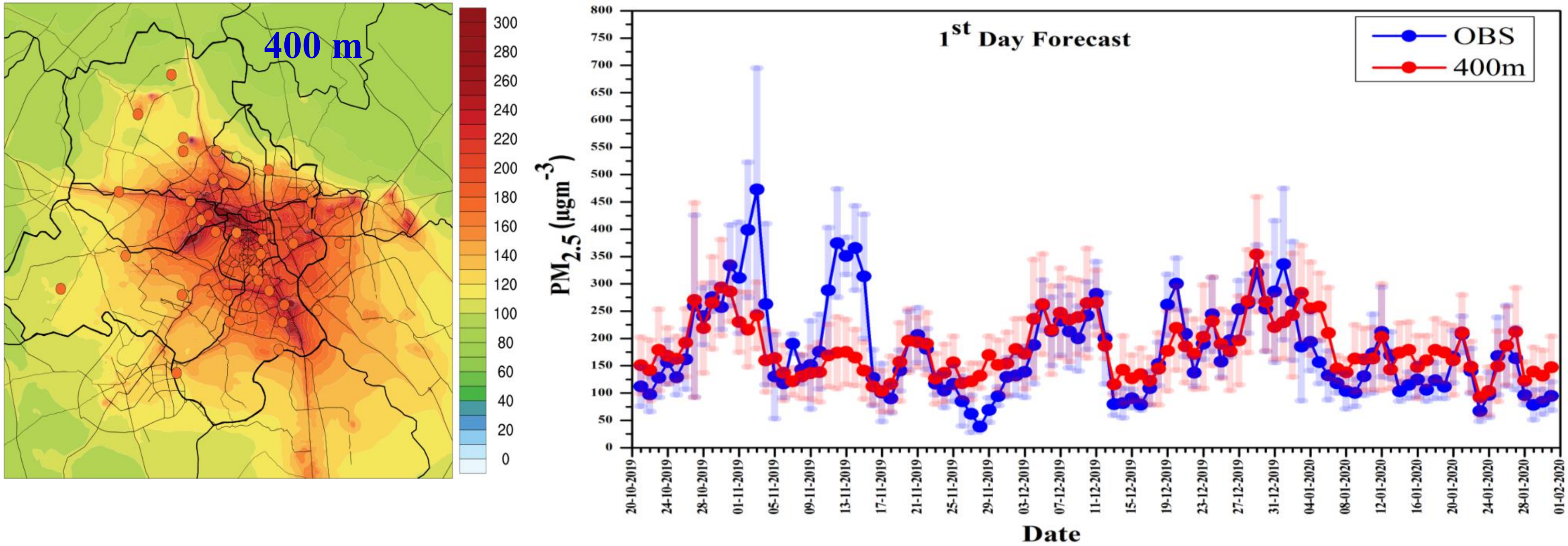

Figure 2: (a) Spatial distribution of averaged $PM_{2.5}$ at 400 m horizontal resolution (from day 1 forecast) overlay with mean $PM_{2.5}$ observed at different monitoring stations across Delhi during 21 October 2019 to 01 February 2020, **(b)** Comparisons between daily mean $PM_{2.5}$ forecast (red) and daily mean $PM_{2.5}$ observations (blue) over Delhi during 21 October 2019 to 01 February 2020 (vertical bar shows the standard deviation).

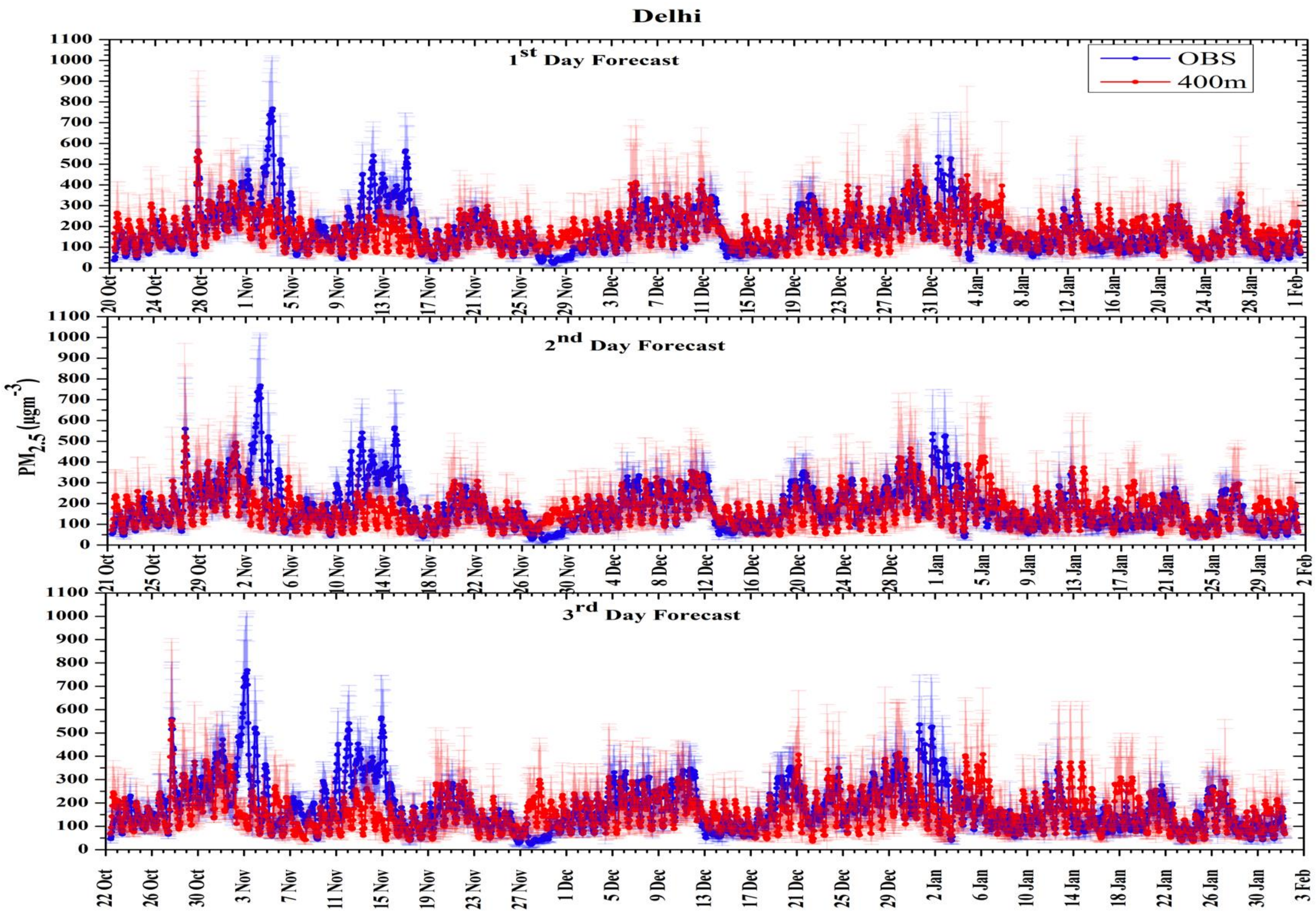

Figure 3: Comparisons between hourly mean $PM_{2.5}$ forecast (red) and hourly mean $PM_{2.5}$ observations (blue) on day one (top), day two (middle) and day three at 400 meter horizontal resolution over Delhi during 21 October 2019 to 01 February 2020 (vertical bar shows the standard deviation).

Table 1: Performance statistics for mean $PM_{2.5}$ forecast and skill score for different forecast AQI category over Delhi during 21 October 2019 to 01 February 2020.

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Statistical performance					
State Variables	Forecast Day	400 meter			
		MB	**NMFB (%)**	**NMFE (%)**	**r**
PM_{25}_hourly	1st day	2.5	1.3	36.3	0.5
	2nd day	-8.4	-4.8	38.1	0.5
	3rd day	-16.8	-9.8	40.5	0.4
PM_{25}_daily	1st day	1.8	1.0	25.6	0.6
	2nd day	-8.8	-5.0	26.7	0.6
	3rd day	-17.3	-10.1	29.5	0.5
PM_{25}_AQI	1st day	21.7	6.5	16.5	0.7
	2nd day	10.4	3.1	16.5	0.6
	3rd day	0.3	0.1	17.8	0.5
Skill score for AQI					
AQI range	Forecast Day	**FAR**	**POD**	**CSI**	**Accuracy**
Unhealthy (poor, very-poor, severe)	1st day	0.11	1.00	0.88	0.88
	2nd day	0.09	0.99	0.90	0.90
	3rd day	0.09	0.98	0.88	0.88
Very Unhealthy (very poor, severe)	1st day	0.28	0.98	0.70	0.72
	2nd day	0.25	0.94	0.71	0.75
	3rd day	0.23	0.89	0.70	0.74
Critical (severe)	1st day	0.35	0.34	0.29	0.82
	2nd day	0.15	0.35	0.33	0.85
	3rd day	0.25	0.21	0.19	0.82

Real-time $PM_{2.5}$ forecast over Delhi: Performance of high resolution (400 m) WRF-Chem model integrated with data assimilation and dynamical downscaling

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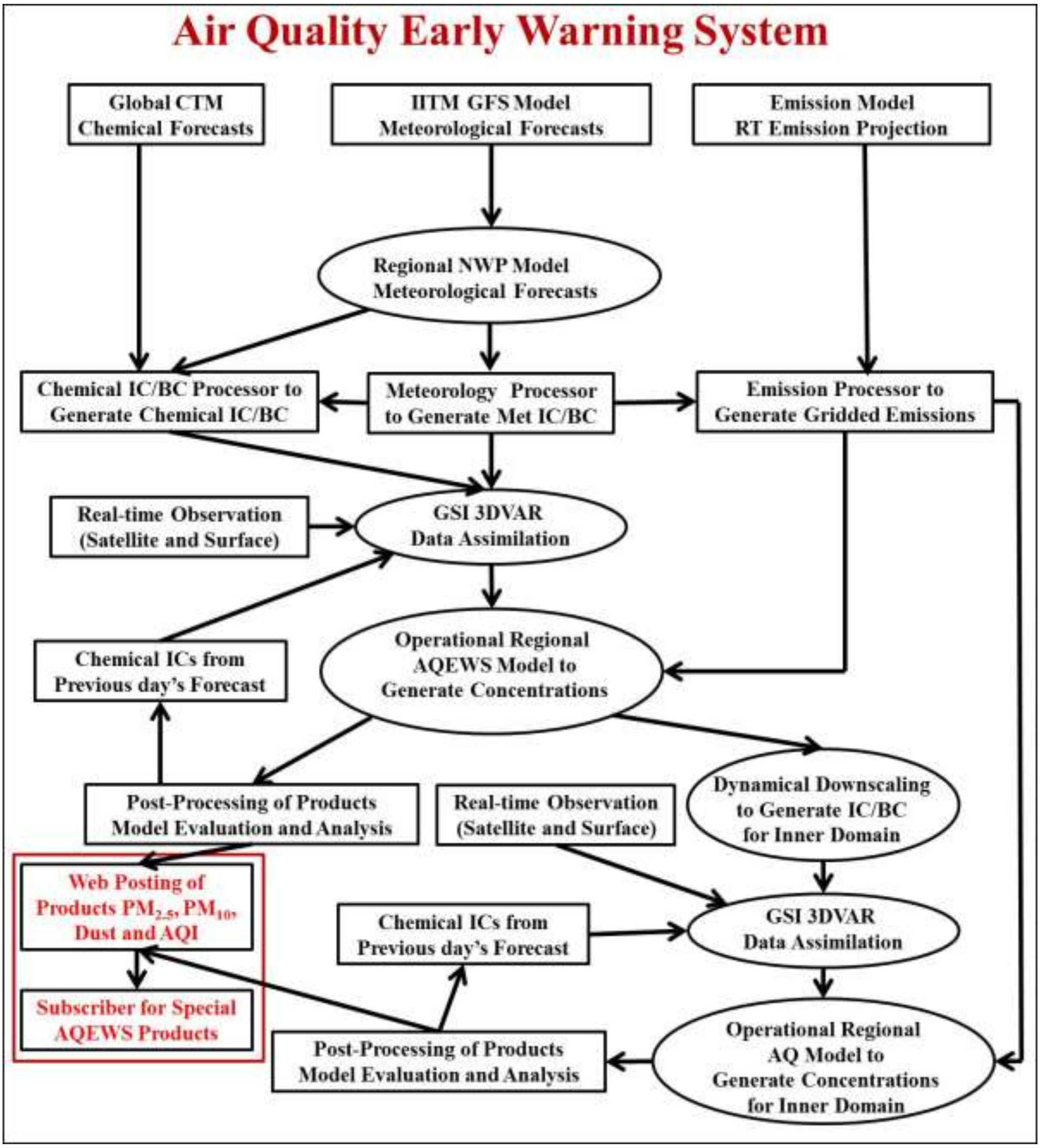

Figure S1: Major system components of air quality early warning system

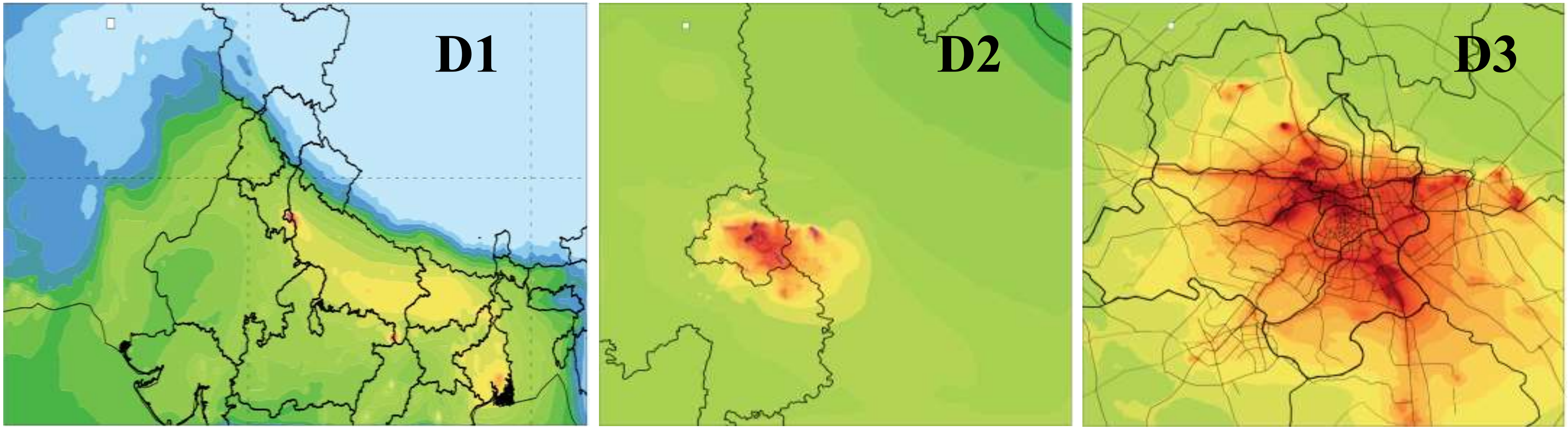

Figure S2: Map of model simulation domain (D1: 10 km horizontal resolution, D2: 2 km horizontal domain and D3: 400 meter horizontal domain)

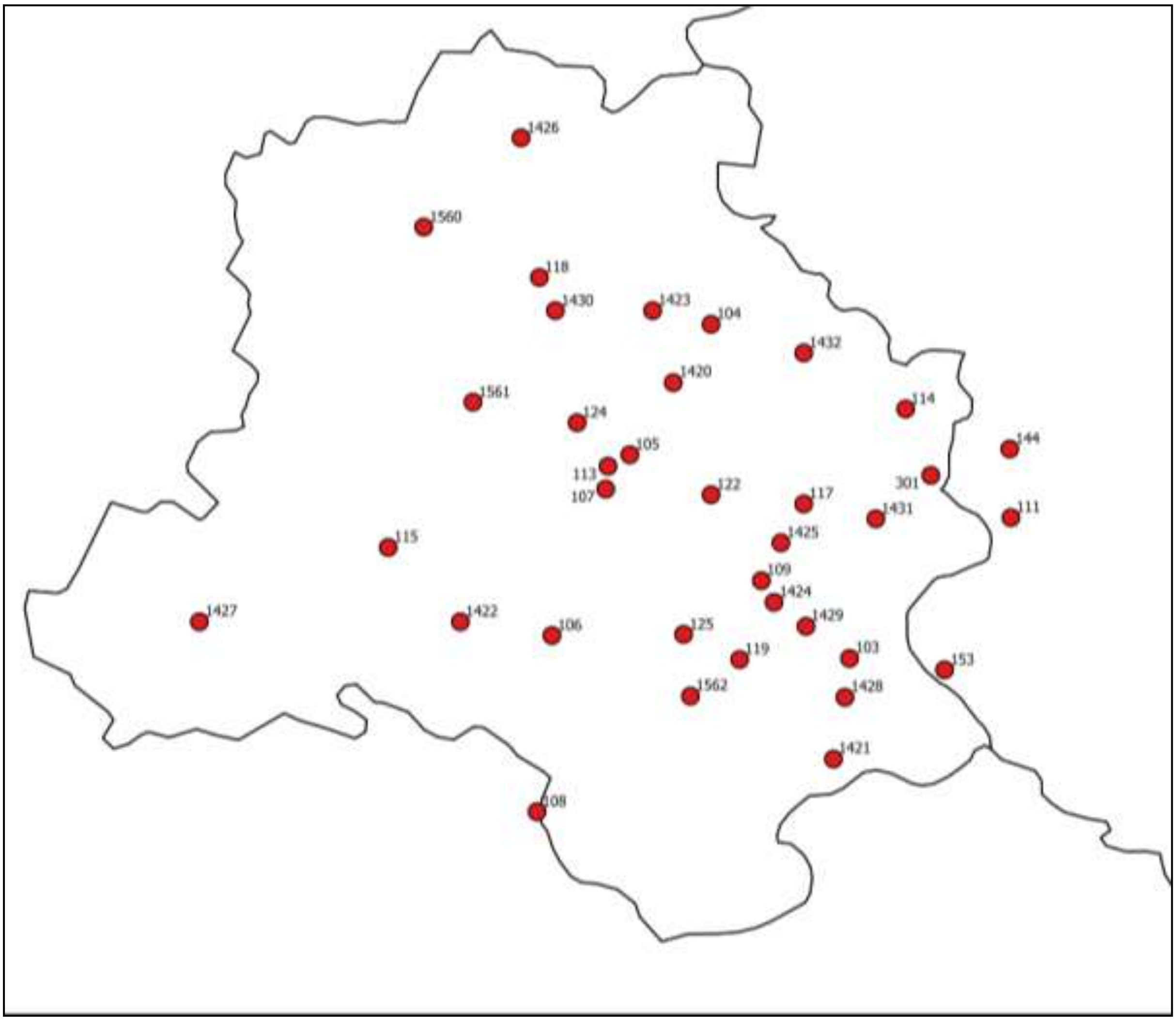

Figure S3: Geographical locations of 37 air quality monitoring stations (stations names associated with the numbers are provided in table ST2)

Figure S4: Spatial emission plots of $PM_{2.5}$ (unit: 10^{10} $kg/m^2/s$) at 400 m horizontal resolution

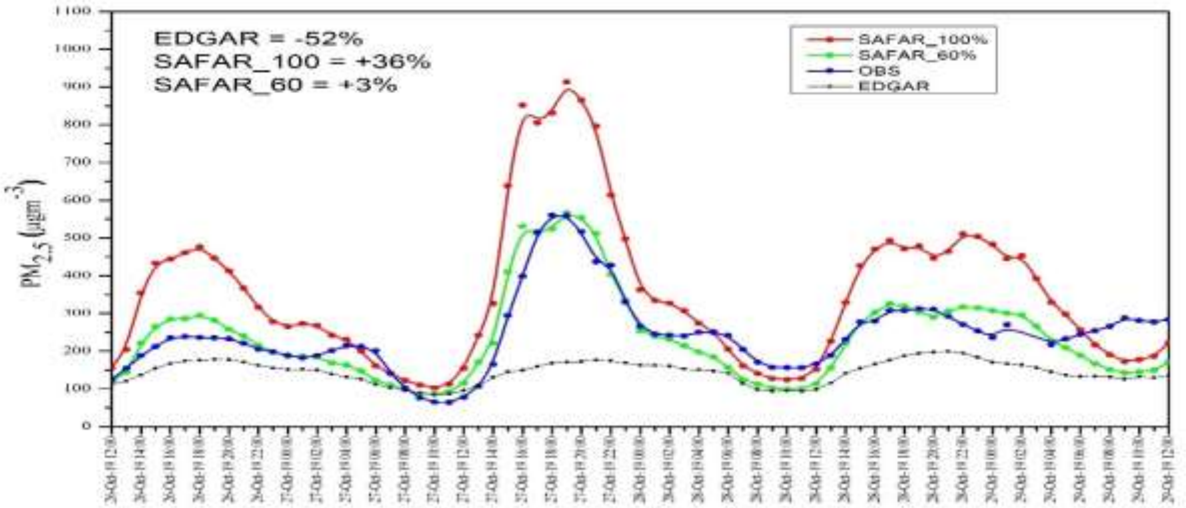

Figure S5: Sensitivity simulations for different emission inventory over Delhi.

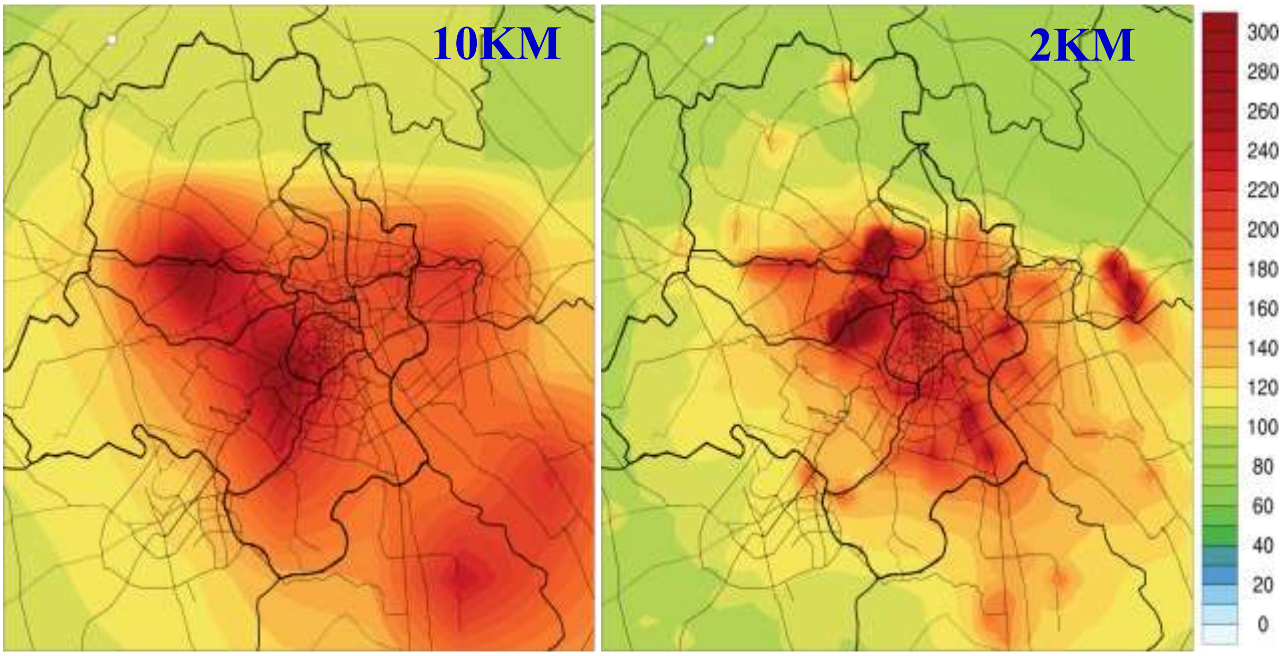

Figure S6: Spatial distribution of average $PM_{2.5}$ of 1st day forecast for 400 meter resolution during 21 October 2019 to 01 February 2020 at 10 km horizontal resolution (left) and 2 Km Horizontal resolution (right).

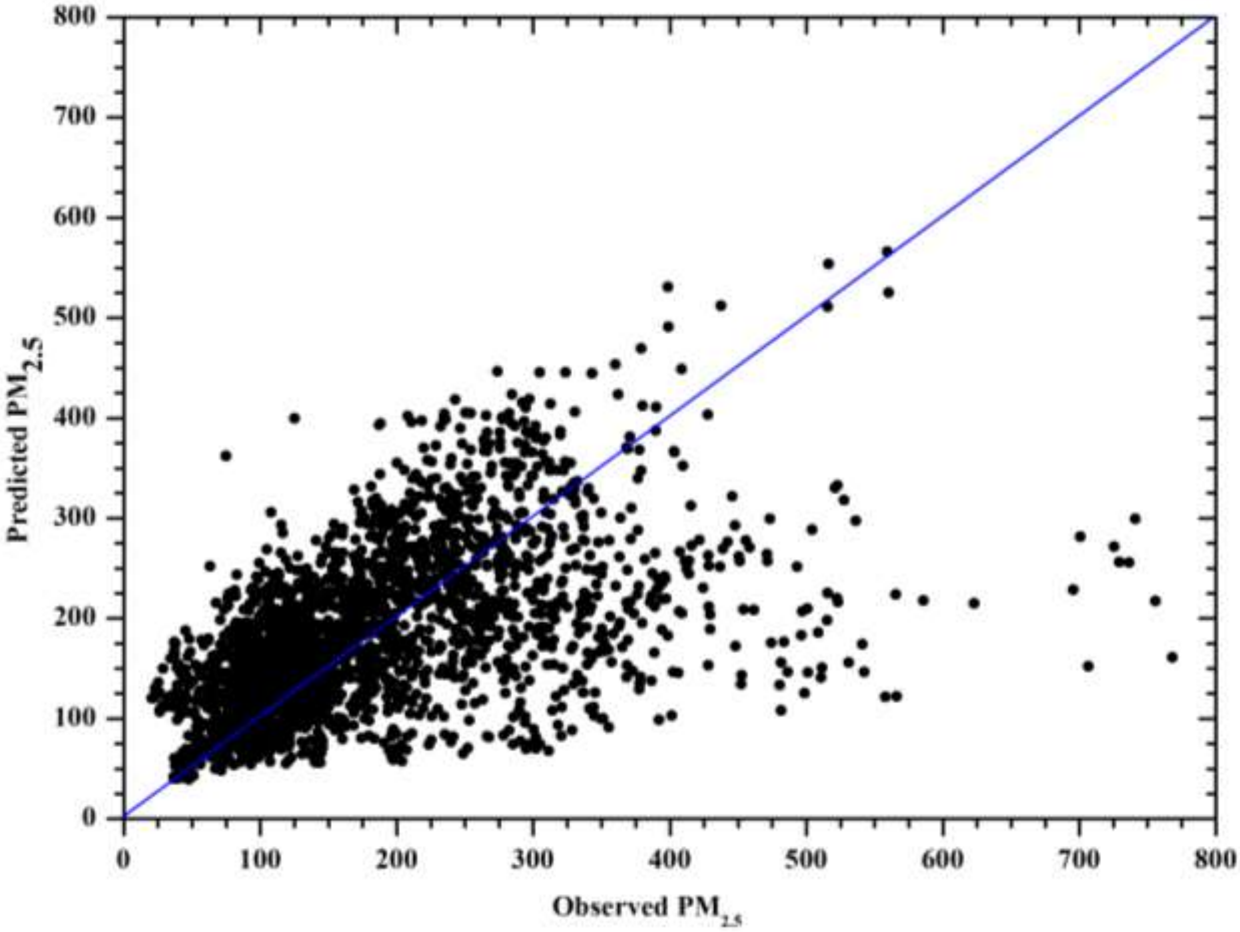

Figure S7: Correlation between hourly mean observed and predicted $PM_{2.5}$ from Delhi.

Table ST1: Selected atmospheric physical and chemical parameterizations

Atmospheric Process	Parameterization
Cloud Microphysics	WRF Single-Moment 6-class scheme (WSM6) (Hong et al., 2006)
Short- and Long-wave radiation	Rapid Radiative Transfer Model for GCMs (Iacono et al., 2008)
Surface Layer	Monin-Obukhov (Janjic Eta)Scheme (Janjic, 1996, 2002)
Land Surface model	Unified Noah Land-surface model (Tewari et al., 2004)
Planetary Boundary Layer	MYNN2.5()
Cumulus	Grell-Freitas ensemble scheme (Grell&Freitas, 2014)
Gas-phase Chemistry	Model for Ozone and Related Tracers (Emmons et al., 2010)
Aerosol Processes	Goddard Global Ozone Chemistry Aerosol Radiation and Transport (GOCART) (Chin et al., 2000)

Table ST2: Performance statistics for simulated $PM_{2.5}$ at different monitoring sites in Delhi during 21 October 2019 to 01 February 2020 at 400 m horizontal resolution

State	Station name	Latitude	Longitude	MB	NMB (%)	RMSE	R
Delhi	CRRI Mathura Road (103)	28.5512005	77.2735737	158.7	87.6	249.9	0.4
	Burari Crossing (104)	28.7256504	77.2011573	-60.2	-31.0	149.5	0.3
	North Campus DU (105)	28.6573814	77.1585447	68.4	40.8	181.6	0.3
	IGI-Airport-T3 (106)	28.5627763	77.1180053	-12.6	-8.1	106.0	0.4
	Pusa IMD (107)	28.639645	77.146262	115.2	83.4	208.1	0.3
	DTU (118)	28.7500499	77.1112615	-95.6	- 45.6	161.2	0.3
	R K Puram (124)	28.674045	77.131023	59.4	37.2	154.0	0.4
	Shadipur (113)	28.6514781	77.1473105	104.4	65.5	177.0	0.6
	NSIT Dwarka (115)	28.60909	77.0325413	-36.1	- 20.7	92.4	0.5
	Mandir Marg (122)	28.636429	77.201067	52.2	29.1	174.3	0.2
	Punjabi Bagh (125)	28.563262	77.186937	-0.5	- 0.2	122.1	0.5
	Sirifort (119)	28.5504249	77.2159377	-12.4	- 6.3	120.4	0.4
	Lodhi Road (109)	28.5918245	77.2273074	34.4	23.3	127.8	0.3
	ITO (117)	28.6316945	77.2494387	20.0	10.7	144.4	0.3
	Anand Vihar (301)	28.646835	77.316032	-52.3	- 25.0	145.2	0.5
	Sector – 62 (111)	28.6245479	77.3577104	-33.5	-17.3	133.8	0.3
	IHBAS-Dilshad-Garden (114)	28.6811736	77.3025234	13.3	8.5	118.5	0.4
	Aya Nagar (108)	28.4706914	77.1099364	-23.8	-15.7	110.8	0.4
	Vasundhara (144)	28.6603346	77.3572563	-31.5	- 14.0	140.5	0.4
	Sector 125 (153)	28.5447608	77.3231257	-14.9	- 7.5	140.9	0.3
	Ashok_Vihar (1420)	28.695381	77.181665	26.1	24.3	79.0	0.2
	DKSS_Stadium (1421)	28.498571	77.264840	-48.0	- 24.5	137.8	0.3
	Dwarka Sector8 (1422)	28.57	77.07				
	Jahangirpuri (1423)	28.732820	77.170633	-81.1	- 35.9	151.5	0.3
	Jawaharlal Nehru Stadium (1424)	28.580280	77.233829	3.0	1.5	116.8	0.5
	MDC National Stadium (1425)	28.611281	77.237738	32.7	19.2	140.0	0.3
	Najafgarh (1427)	28.570173	76.933762	46.1	85.3	59.3	0.1
	Narela (1426)	28.822836	77.101981	-49.4	- 38.8	66.8	0.1
	Nehru Nagar (1429)	28.567890	77.250515	-9.2	- 3.8	145.3	0.5
	Okhla Phase2 (1428)	28.530785	77.271255	17.4	14.7	77.6	0.2
	Patparganj (1431)	28.623748	77.287205	28.7	16.0	122.5	0.4
	Rohini (1430)	28.732528	77.119920	-88.6	- 39.1	163.0	0.4
	Sonia Vihar (1432)	28.710508	77.249485	-44.6	- 25.8	114.3	0.3
	Sri_Aurbindo_Marg (1562)	28.531346	77.190156	2.6	3.1	53.5	0.1
	Mundak (1561)	28.684678	77.076574	19.0	18.8	50.8	0.6
	New_collectorate (1569)	28.974801	77.213357	-83.3	- 46.4	142.2	0.4
	New_mandi (1550)	29.4723508	77.7194031	-65.0	- 44.9	109.6	0.4
	Bawana (1560)	28.776200	77.051074	-92.6	- 41.9	163.4	0.4

Table ST3: Model performance goals used to evaluate the model performance for $PM_{2.5}$ (Morris et al., 2005)

Fractional Bias	Fractional Error	Comment
$\leq \pm 15\%$	$\leq 35\%$	A level of model performance that would be considered excellent
$\leq \pm 30\%$	$\leq 50\%$	A level of model performance that would be considered good
$\leq \pm 60\%$	$\leq 75\%$	A level of model performance that would be considered average and hope each PM species could meet for regulatory modeling
$> \pm 60\%$	$>75\%$	At or exceeding this level of performance indicates fundamental problems with the modeling system

Table ST4: AQI category and corresponding break-point concentrations ranges for PM2.5 based on National Ambient Air Quality Standard (NAAQS)**.**

AQI Category	AQI	$PM_{2.5}$ Concentration range
Good	0 - 50	0 - 30
Satisfactory	51 - 100	31 - 60
Moderately	100 - 200	61 - 90
Poor	201 - 300	91 - 120
Very poor	301 - 400	121 - 250
Severe	401 +	250+

Table ST5: Performance statistics of different $PM_{2.5}$ AQI forecast category

State	PM_{25} AQI Category	Variables	10km			2km			400 meter		
			MB	**NMFB (%)**	**NMFE (%)**	**MB**	**NMFB (%)**	**NMFE (%)**	**MB**	**NMFB (%)**	**NMFE (%)**
Delhi	Poor (201-300)	1st day	51.1	18.4	19.3	66.2	23.2	23.3	62.9	22.1	22.3
		2nd day	30.4	11.4	20.8	56.1	20.0	22.6	53.6	19.2	22.2
		3rd day	16.3	6.2	23.2	42.4	15.4	20.9	44.6	16.2	20.2
	Very Poor (301-400)	1st day	4.2	1.2	6.4	12.3	3.5	7.4	8.2	2.3	6.8
		2nd day	-17.7	-5.3	9.1	0.2	0.1	6.7	-2.7	-0.8	6.9
		3rd day	-27.5	-8.3	11.4	-13.7	-4.0	8.9	-13.4	-3.9	8.7
	Severe (401-above)	1st day	-47.1	-11.1	15.6	-55.5	-13.3	16.2	-58.0	-13.9	16.3
		2nd day	-89.0	-22.1	22.2	-70.2	-17.1	17.5	-70.8	-17.2	17.8
		3rd day	-105.0	-26.7	26.7	-86.2	-21.4	21.8	-83.6	-20.7	20.9

Table ST6: A contingency table and equations used to calculate the different skill score for different category of AQI forecast.

		Observation	
		YES	**NO**
Forecast	**YES**	**a**	**b**
	NO	**c**	**d**

Statistic name	What it measures	Equation	unit	How to interpret
Accuracy (A)	Percent of forecasts thatcorrectly predicted the event ornon-event.	A=(a+d)/(a+b+c+d) *100	%	Higher numbers are better
False Alarm Rate (FAR)	The percent of times a forecastof high pollution did notactually occur.	FAR = (b/(a+b)) *100	%	Smaller values are best
Probability of Detection (POD) or Hit rate	Ability to predict highpollutionevents (i.e., thepercentage of forecasted highpollutionevents that actuallyoccurred).	POD = (a/(a+c)) * 100	%	Higher numbers are best
Critical Success Index (CSI), also called Threat Score	How well the high-pollutionevents were predicted. Usefulfor evaluating rarer events likehigh-pollution days. It is not affected by a large number ofcorrectly forecasted, lowpollutionevents.	CSI = (a/(a+b+c)) * 100	%	Higher numbers are best