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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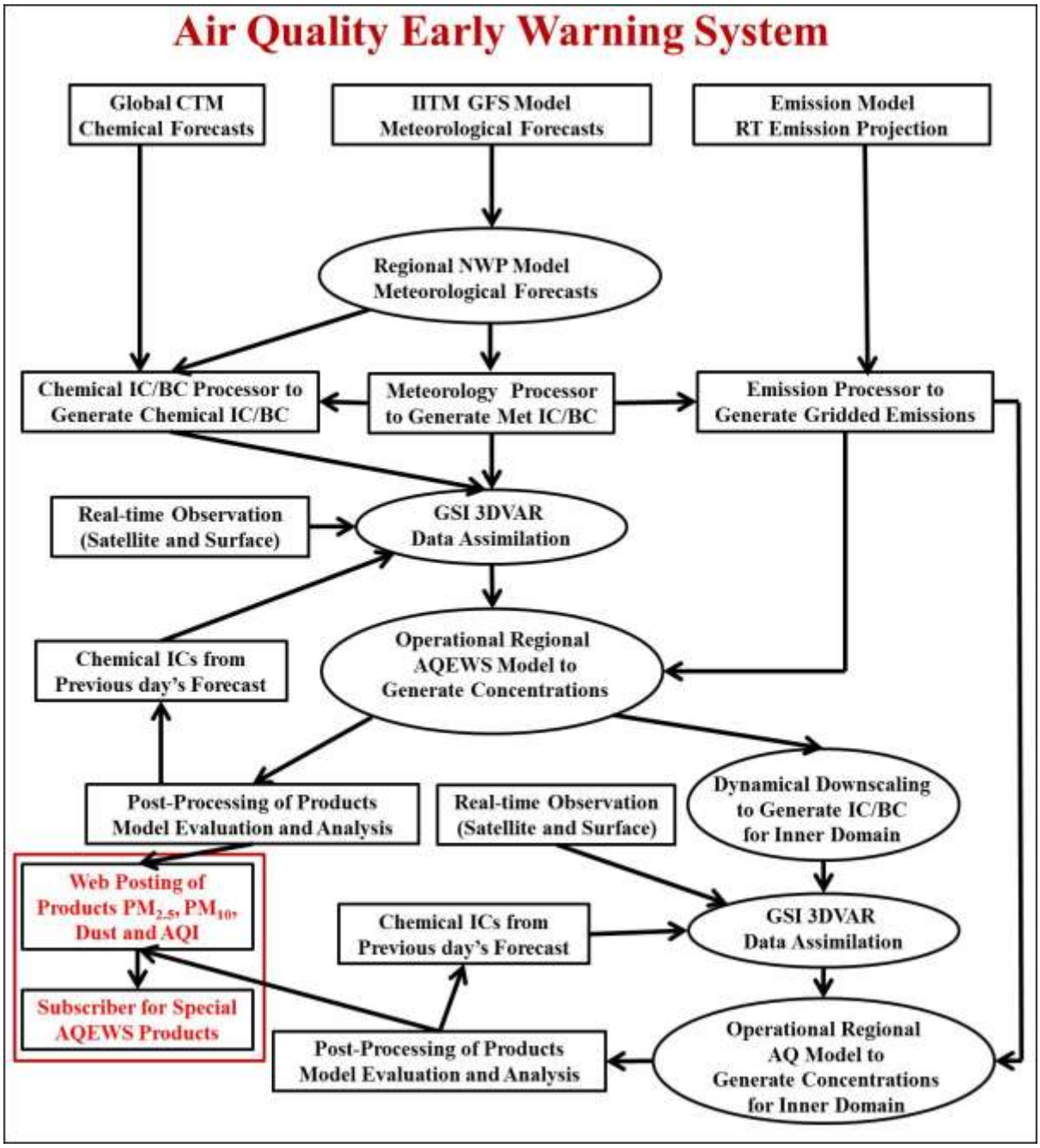

Figure S1: Major system components of air quality early warning system

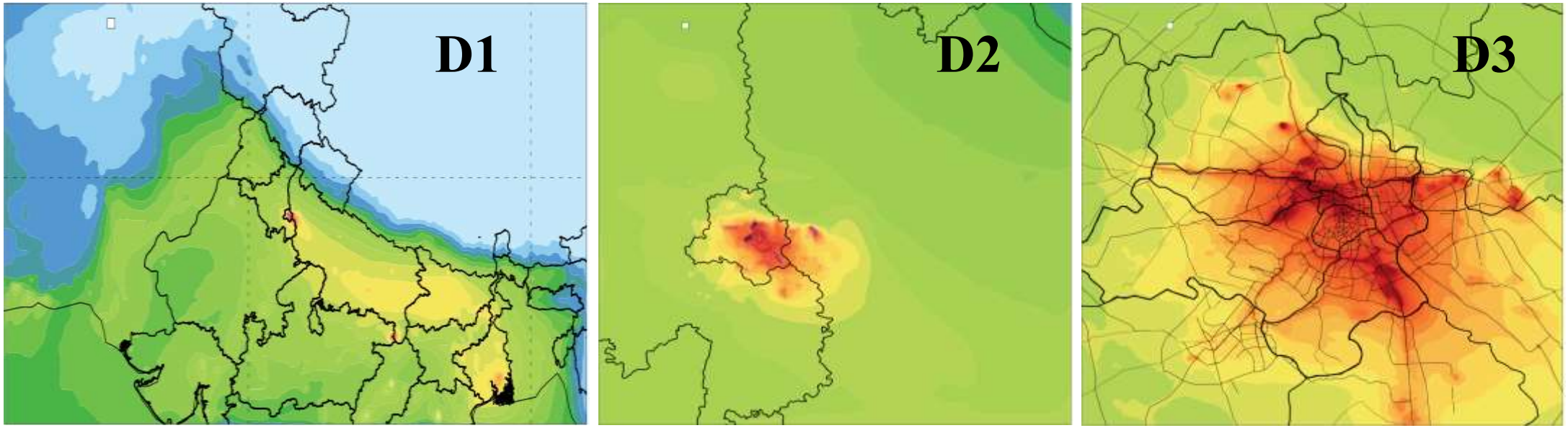

Figure S2: Map of model simulation domain (D1: 10 km horizontal resolution, D2: 2 km horizontal domain and D3: 400 meter horizontal domain)

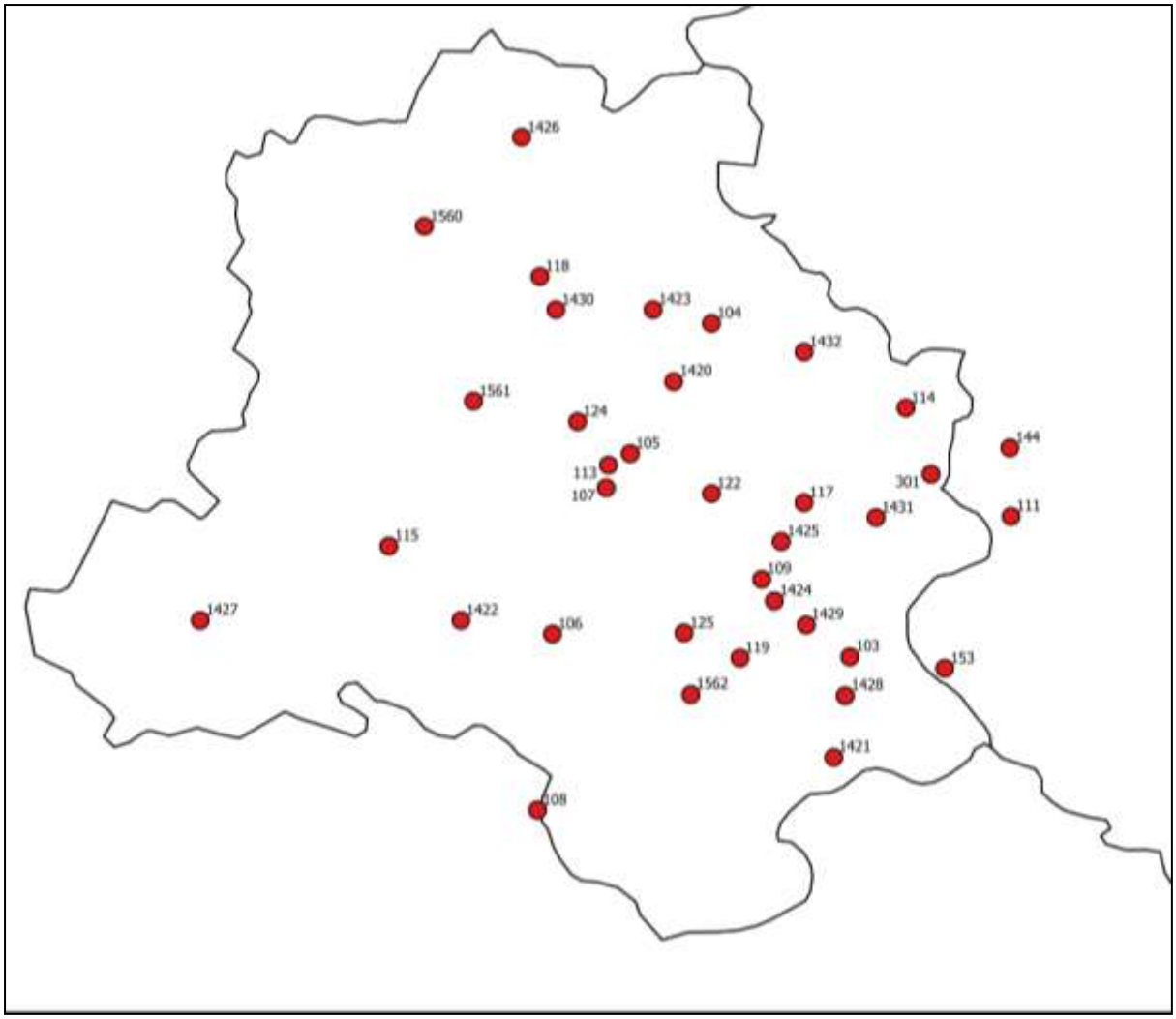

Figure S3: Geographical locations of 37 air quality monitoring stations (stations names associated with the numbers are provided in table ST2)

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

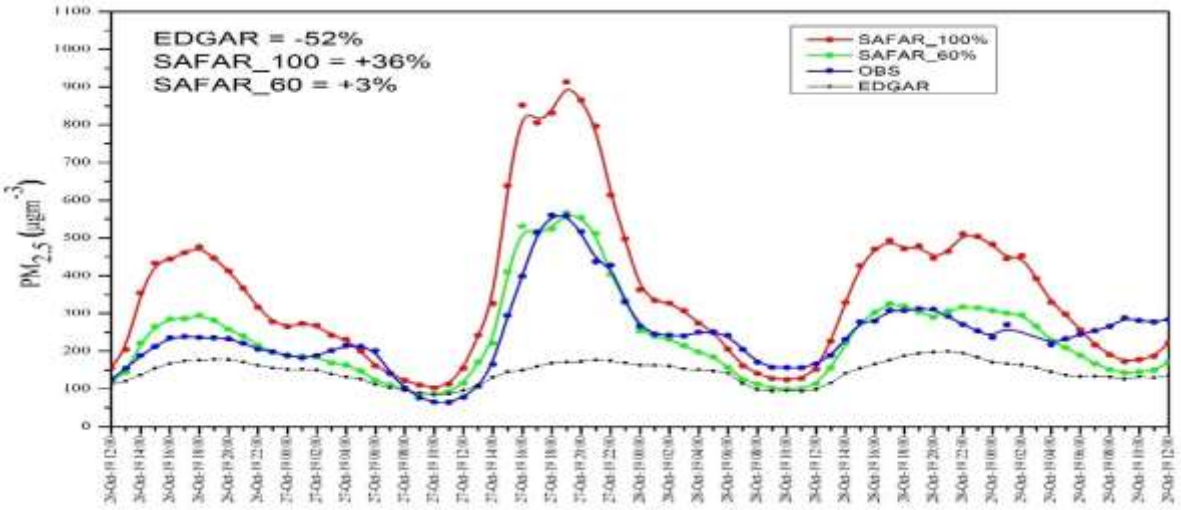

Figure S5: Sensitivity simulations for different emission inventory over Delhi.

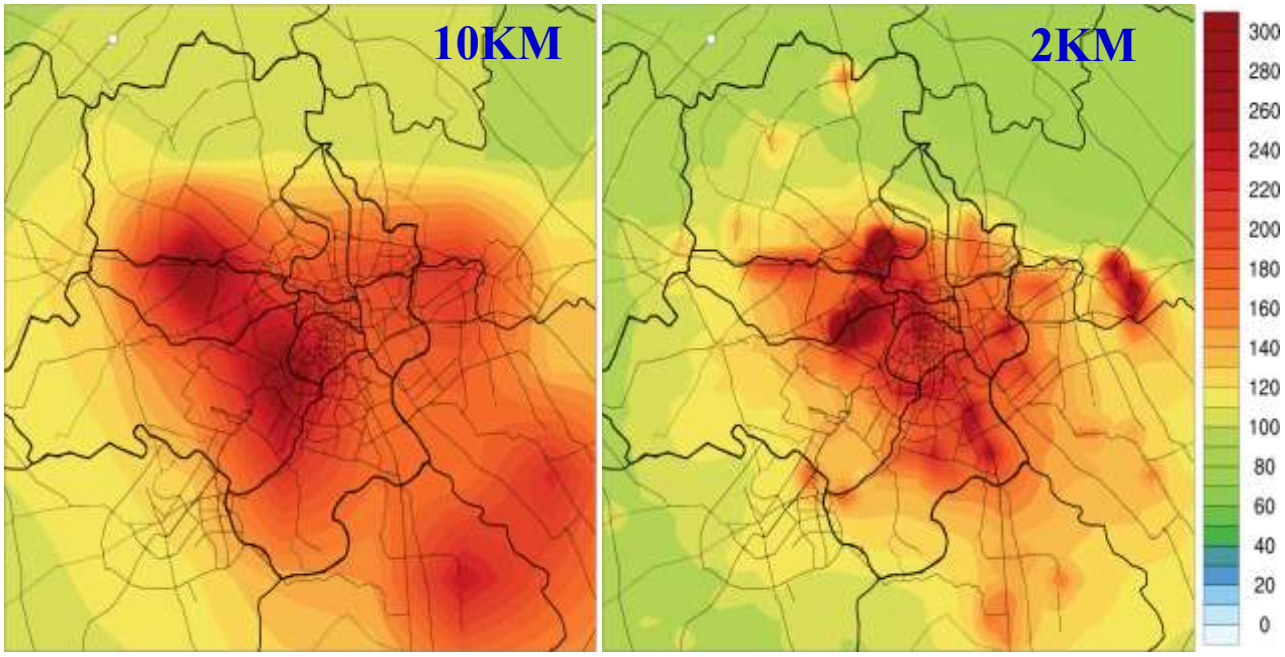

Figure S6: Spatial distribution of average $PM_{2.5}$ of 1st day forecast for 400 meter resolution during 21 October 2019 to 01 February 2020 at 10 km horizontal resolution (left) and 2 Km Horizontal resolution (right).

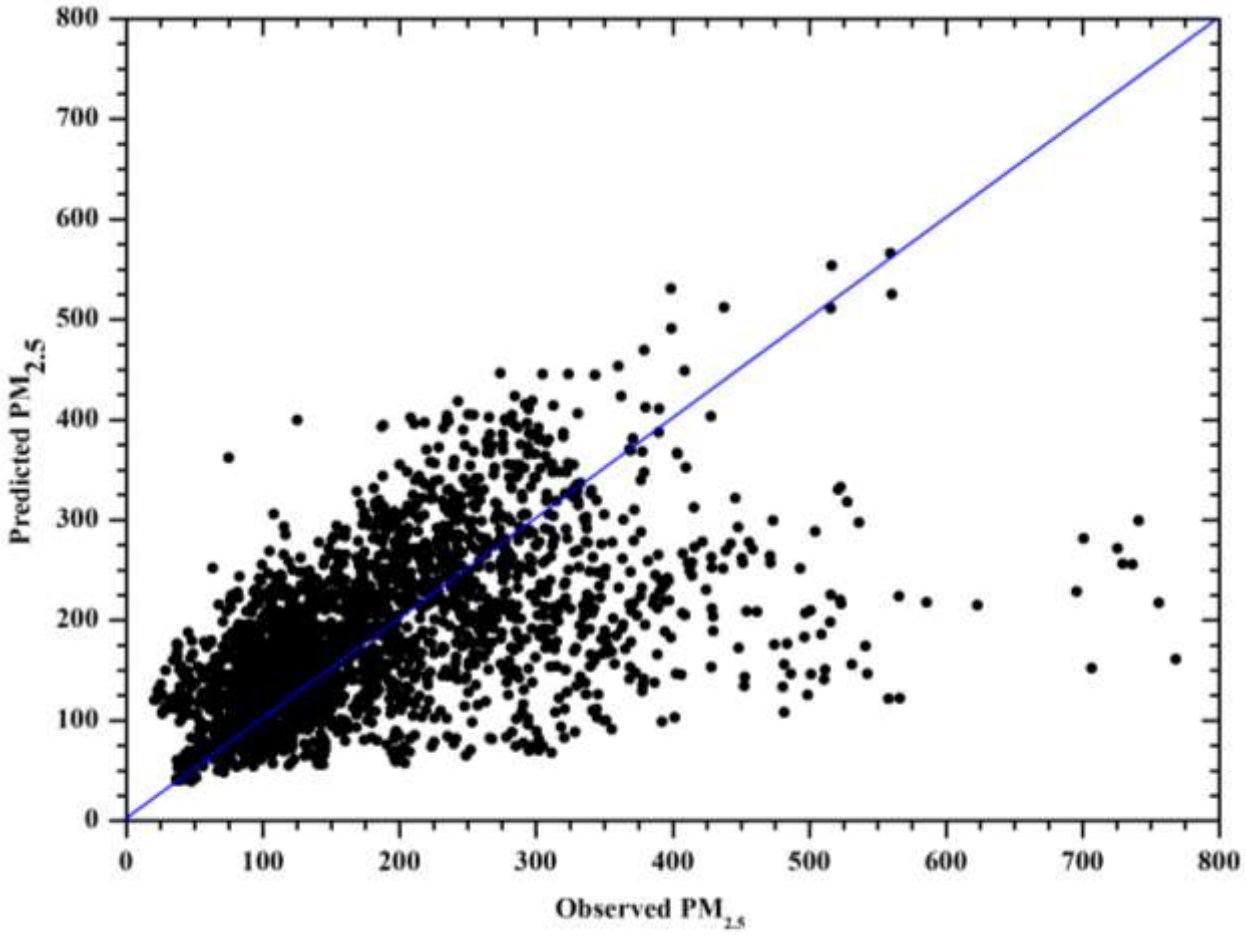

Figure S7: Correlation between hourly mean observed and predicted $PM_{2.5}$ from Delhi.

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
≤ ± 15%	≤35%	A level of model performance that would be considered excellent
≤ ± 30%	≤50%	A level of model performance that would be considered good
≤ ± 60%	≤75%	A level of model performance that would be considered average and hope each PM species could meet for regulatory modeling
> ± 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.

Forecast \ Observation	YES	NO
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