Supplementary Material

Evaluation of WRF-Chem simulated meteorology and aerosols over northern India during the severe pollution episode of 2016

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Table S1. WRF-Chem model set-up and selected parametrization schemes.

WRF-Chem Configuration	Description
Microphysics	Morrison double-moment scheme
Longwave radiation	Rapid Radiative Transfer Model (RRTM) longwave scheme
Shortwave radiation	RRTMG shortwave scheme
Boundary-layer physics	Mellor–Yamada Nakanishi and Niino 2.5 level (MYNN2)
Convective parameterisation	Grell 3D ensemble scheme
Land-surface interactions	Unified Noah land-surface model with urban canopy model
Surface layer	MYNN surface layer

Table S2. Details of open-access observation datasets used in this study for model evaluation.

Dataset / Network	Access link (Last access: 30 December 2022)
IEM-ASOS Network, Iowa Environmental Mesonet- Automated Surface Observing System	https://mesonet.agron.iastate.edu/request/download.phtml?network=IN__ASOS
RAOB, Radiosonde observations University of Wyoming database	http://weather.uwyo.edu/upperair/sounding.html
MERRA-2, Modern-Era Retrospective analysis for Research and Applications, Version 2	https://gmao.gsfc.nasa.gov/reanalysis/MERRA-2/
MODIS, Moderate Resolution Imaging Spectroradiometer	https://ladsweb.modaps.eosdis.nasa.gov/search
AERONET, AErosol RObotic NETwork	https://aeronet.gsfc.nasa.gov/
CPCB, Central Pollution Control Board	https://openaq.org/

Table S3: The statistical metrics used for model-observation comparison in this study

Mean Bias (MB)	$\dfrac{1}{n}\sum_{1}^{n}(M-O)$
Normalized mean bias (NMB)	$\dfrac{\sum_{1}^{n}(M-O)}{\sum_{1}^{n}(O)}$
Mean absolute error (MAE)	$\dfrac{1}{N}\sum_{i=1}^{N}\left|M_i-O_i\right|$
Root mean square error (RMSE)	$\sqrt{\dfrac{\sum_{1}^{n}(M-O)^2}{n}}$
Pearson's Correlation coefficient (r)	$r=\dfrac{\sum_{i=0}^{N}(M_i-M)(O_i-O)}{\sqrt{\sum_{i=1}^{N}(M_i-\overline{M})^2\sum_{i=0}^{N}(O_i-\overline{o})^2}}$

Site Name	Longitude	Latitude	Elevation / m
Ahmedabad	72.63	23.08	55.0
Baroda	73.27	22.33	44.7
Bhopal	77.34	23.29	522.7
Bhaunagar	72.19	21.75	11.3
Indore	75.80	22.72	563.1
Jabalpur	79.95	23.20	402.2
Nagpur	79.05	21.09	310.0
Porbandar	69.66	21.65	7.0
Rajkot	70.78	22.31	136.9
Udaipur	73.90	24.62	508.4
Agartala	91.24	23.89	16.0
Baghdogra	88.32	26.63	126.0
Shillong	91.98	25.70	892.2
Bhubaneswar	85.82	20.24	46.0
Guwahati	91.59	26.11	54.0
Gaya	84.95	24.74	116.0
Imphal	93.90	24.76	781.0
Jamshedpur	86.17	22.81	151.7
Aizwal	92.62	23.84	427.6
Lilabari	94.10	27.30	101.0
Dimapur	93.77	25.88	147.3
Ranchi	85.32	23.31	652.0
Raipur	81.74	21.18	316.0
Kulu	77.17	31.83	1080.7
Dehra Dun	78.18	30.19	547.9
Kangra	76.26	32.17	762.2
Gwalior	78.25	26.23	207.0
Jodhpur	73.02	26.30	294.2
Jaipur	75.81	26.82	390.0
Jammu	74.84	32.69	288.4
Kota	75.85	25.16	285.7
Leh	77.55	34.14	3257.8
Shimla	77.07	31.08	1535.5
Srinagar	74.77	33.99	1666.0
Delhi	77.1	28.6	233.0
Ludhiaha	76.0	30.9	255.7
Lucknow	80.9	26.8	128.0
Varanasi	82.9	25.5	83.0
Kolkata	88.4	22.7	6.0
Cooch-behar	89.5	26.3	46.6
Gorakhpur	83.4	26.8	77.0
Patina	85.1	25.6	60.0
Agra	78.0	27.2	169.0
Amritsar	74.9	31.6	234.0
Chandigarh	76.8	30.7	316.4
Delhi	77.2	28.6	215.2

Table S4. Locations and elevations of the ASOS measurement sites used for meteorology evaluation.

Table S5. Locations of the CPCB measurement sites used for $PM_{2.5}$ evaluation.

	City	Location	Latitude	Longitude
1	Agra	Sanjay Palace	27.20	78.01
2	Delhi	Delhi Technological University	28.74	77.12
3	Delhi	Income Tax Office	28.62	77.25
4	Delhi	R K Puram	28.56	77.17
5	Delhi	Anand Vihar	28.65	77.32
6	Delhi	Mandir Marg	28.63	77.20
7	Delhi	US Diplomatic Post: New Delhi	28.64	77.22
8	Delhi	Punjabi Bagh	28.67	77.12
9	Gaya	Collectorate - Gaya - BSPCB	24.75	84.94
10	Gurgaon	Vikas Sadan Gurgaon - HSPCB	28.45	77.03
11	Jaipur	VK Industrial Area Jaipur - RSPCB	26.97	75.77
12	Jodhpur	Collectorate Jodhpur - RSPCB	26.29	73.04
13	Kanpur	Nehru Nagar	26.47	80.33
14	Kolkata	US Diplomatic Post: Kolkata	22.55	88.35
15	Lucknow	Central School	26.85	81.00
16	Muzaffarpur	Collectorate - Muzaffarpur - BSPCB	26.08	85.41
17	Panchkula	Sector 6 Panchkula - HSPCB	30.71	76.85
18	Patna	IGSC Planetarium Complex - Patna - BSPCB	25.36	85.08
19	Rohtak	MD University, Rohtak - HSPCB	28.88	76.62
20	Varanasi	Ardhali Bazar	25.35	82.98
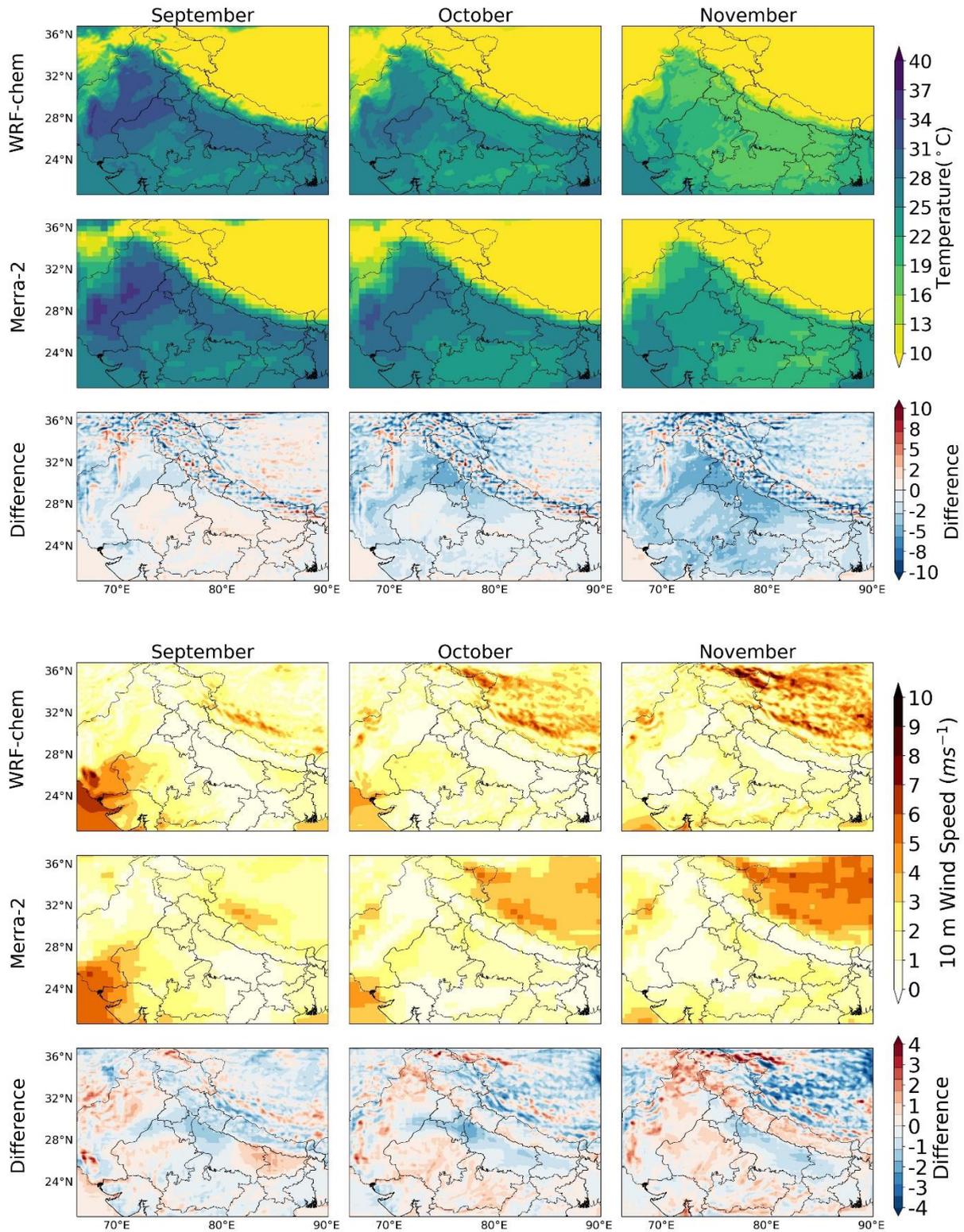
Figure S1. Comparisons of spatial distribution of monthly mean a) 2-m temperature and b) 10-m wind speed between WRF-Chem and MERRA-2 data for September to November 2016. The bottom row in a) and b) show the WRF-Chem minus MERRA-2 absolute differences.
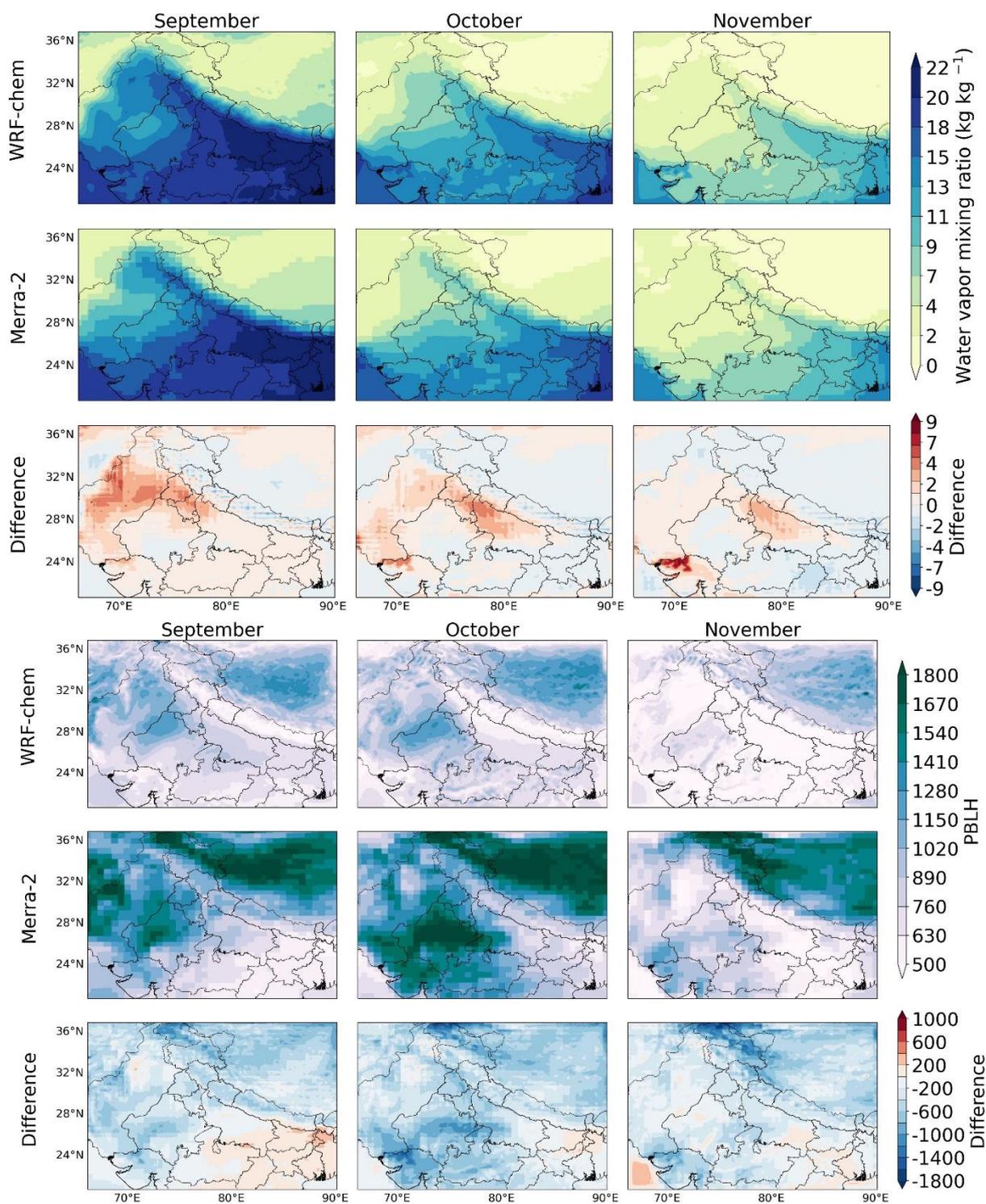
Figure S2. Comparisons of spatial distribution of monthly mean a) surface water vapor mixing ratio and b) PBLH between WRF-Chem and MERRA-2 data for September to November 2016. The bottom row in a) and b) show the WRF-Chem minus MERRA-2 absolute differences.
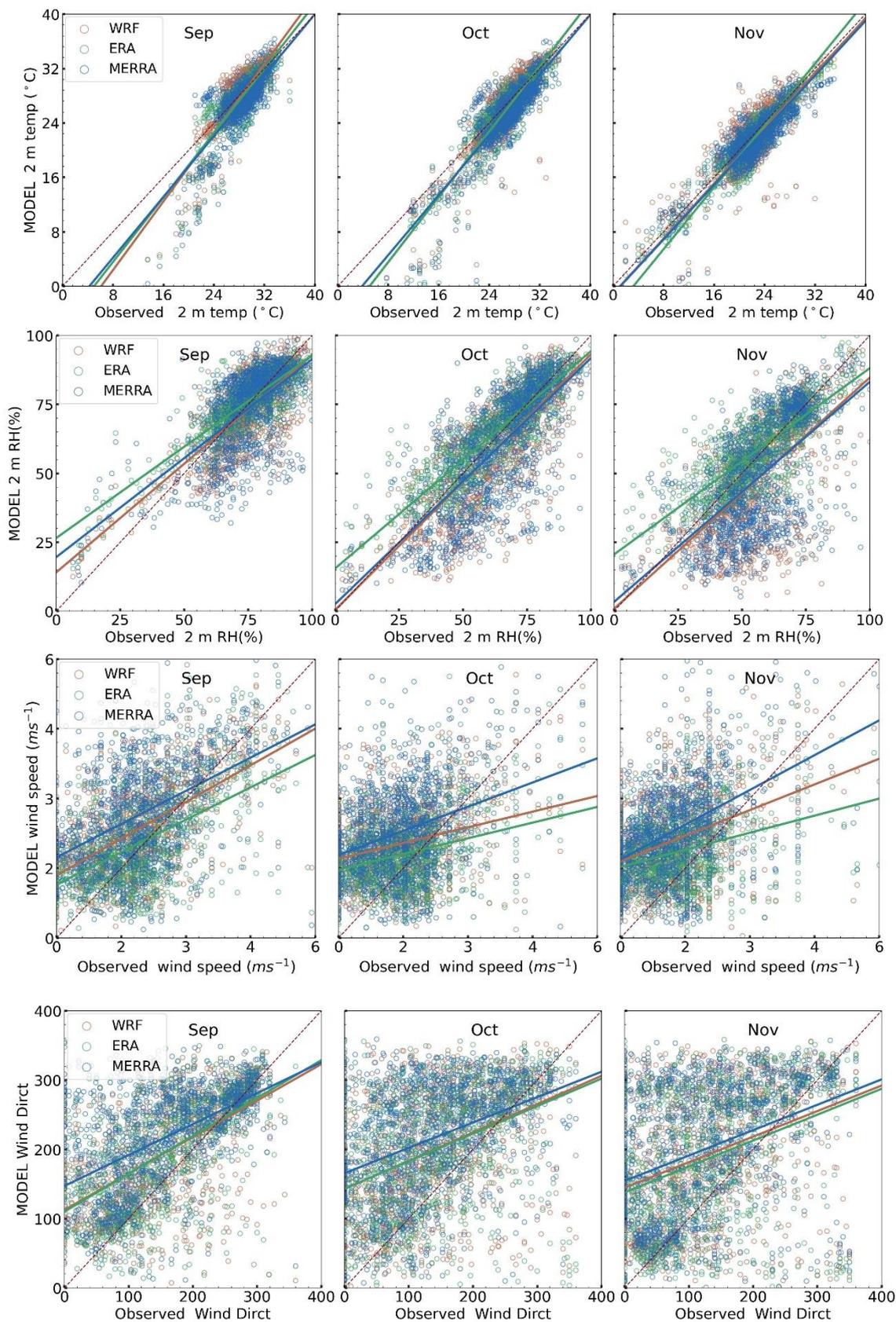
Figure S3. Scatter plots of daily mean measured and modelled surface meteorology variables derived from ERA-5, MERRA-2 and WRF-Chem across the 49 ASOS measurement sites for each of the 3 months of the study period: 2 m temperature, relative humidity (%), and wind speed (m s^{-1}). The 1:1 line is shown as red dashed.
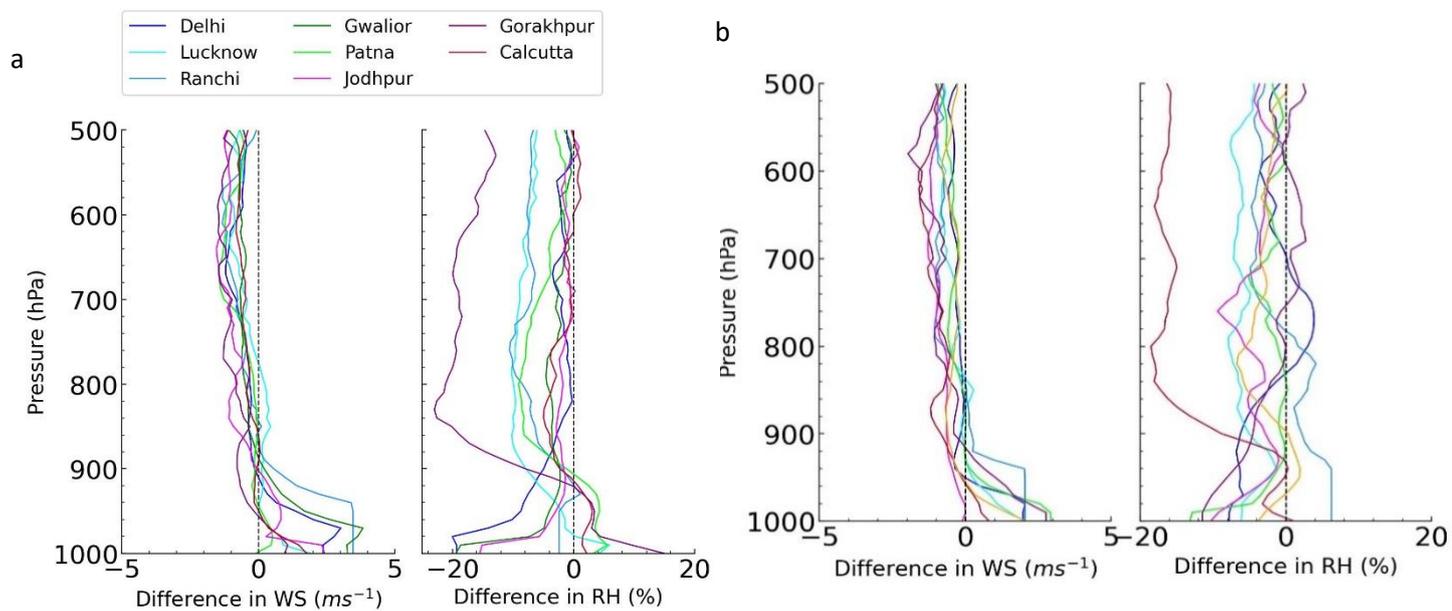
Figure S4. Difference between model and radiosonde vertical profiles at all RAOB sites at a) 00 UTC (5.30 IST) and b) 12 UTC (17.30 IST) for wind speed, WS (first panel) and relative humidity, RH (right panel).
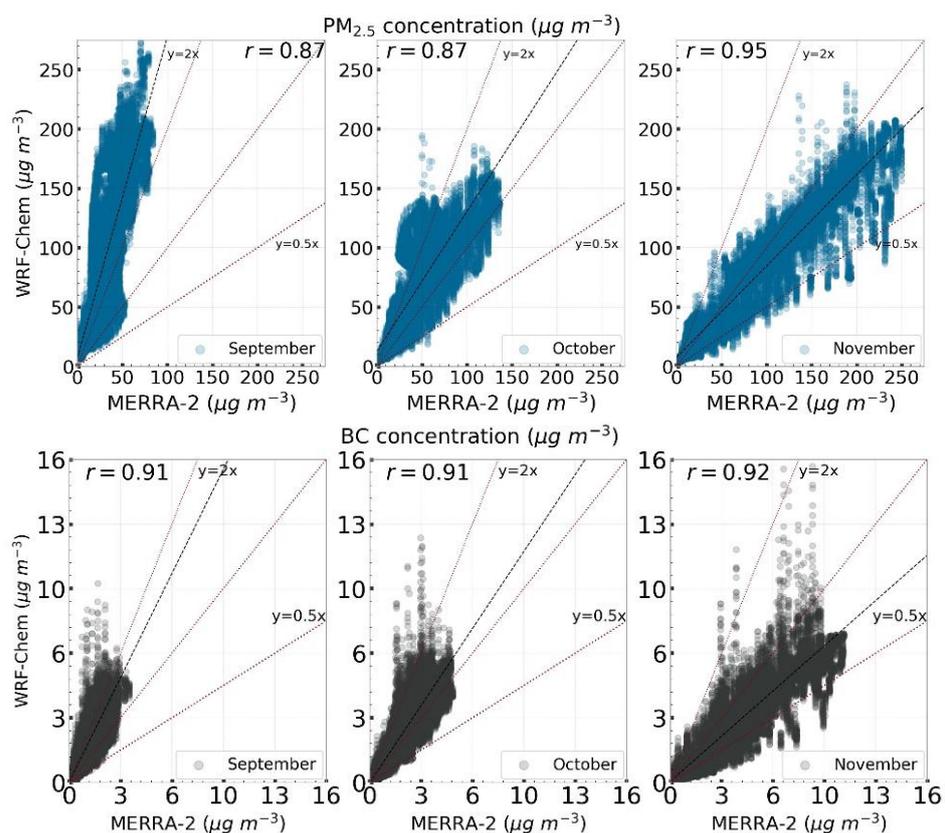
Figure S5. Scatter plots for comparisons of spatial distribution of monthly mean concentrations (µg m^{-3}) of PM$_{2.5}$ (top) and black carbon (bottom) from the WRF-Chem model and MERRA-2 from September to November 2016. The 2:1, 1:1 and 1:2 lines (red dashed lines), the best-fit line (black line) and Pearson's correlation coefficient r are also shown for each month.
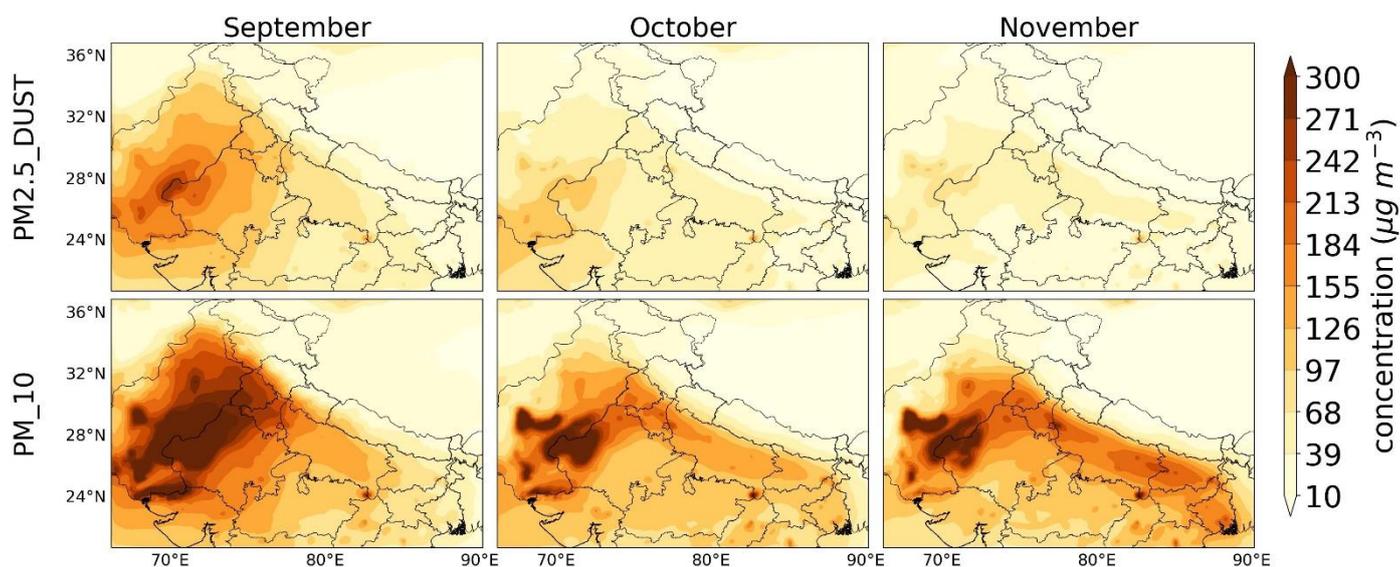
Figure S6. Spatial distributions of modelled monthly mean concentrations of the dust component of PM$_{2.5}$ (top row) and of PM$_{10}$ (bottom row) for September to November 2016.