

Toward Reliable Air Quality Simulations over India: Optimizing WRF-Chem through Comprehensive Sensitivity Analysis of Meteorology, Physical Parameterizations, and Emission Inventories

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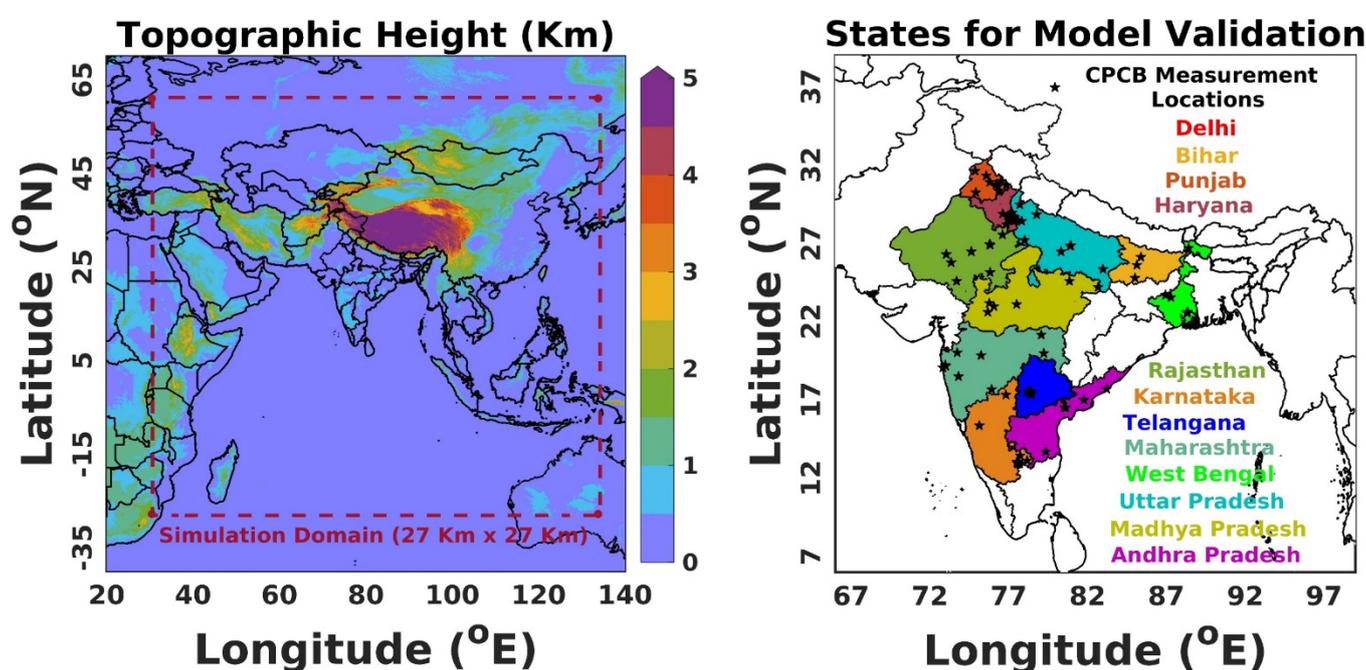


Figure S1. WRF-Chem simulation domain overlaid with Topographic Height (first panel) and different Indian states that have been used for validating the model performance (second panel) are shown, overlaid with CPCB measurement sites available for 2018, 2019. This setup was used to examine the WRF-Chem model performance with multiple sensitivity choices over the Indian region.

Table S1. Summary of WRF-Chem model sensitivity simulations setup details.

SI No.	WRF-Chem model Configuration Details		Simulation Name
Meteorology Sensitivity Simulations			Common Model Configurations
1	ERA5	YSU PBL, Purdue Lin Microphysics, SMOG-COALESCCE Emission, MOZART – MOSAIC, No Nudging	Control
2	NCEP CFSv2		CFSWRF
3	NCEP GDAS		GDASWRF
PBL Sensitivity Simulations			
1	YSU Scheme	ERA5 Meteorology, Purdue Lin Microphysics, SMOG-COALESCCE Emission, MOZART – MOSAIC, No Nudging	Control
4	MYJ Scheme		MYJWRF
5	MYNN3 Scheme		MYNWRF
Microphysics Sensitivity Simulations			
1	Purdue Lin Scheme	ERA5 Meteorology, YSU PBL, SMOG-COALESCCE Emission, MOZART – MOSAIC, No Nudging	Control
6	New Thompson Scheme		THOMWRF
7	Morrison Double-Moment Scheme		MDMWRF
Grid Nudging Approach Sensitivity Simulations			
8	Grid Nudging for Winds, Temperature, and Water Vapor from ERA5	ERA5 Meteorology, YSU PBL, Purdue Lin Microphysics, SMOG-COALESCCE Emission, MOZART – MOSAIC, Whole Atmosphere Nudging, Nudging Coeff. 0.0003 s^{-1}	Nudged03
Chemical Mechanism Sensitivity Simulations			
9	CBMZ – MOSAIC (4 bins, DMS, Aqueous)	ERA5 Meteorology, YSU PBL, Purdue Lin Microphysics, SMOG-COALESCCE Emission, Whole Atmosphere Nudging, Nudging Coeff. 0.0003 s^{-1}	CBMZWRF
8	MOZART – MOSAIC (4 bins, VBS, Aqueous)		Nudged03
Emission Inventory Sensitivity Simulations			
10	CMIP6 (2014)	ERA5 Meteorology, YSU PBL, Purdue Lin Microphysics, MOZART – MOSAIC, Whole Atmosphere Nudging, Nudging Coeff. 0.0003 s^{-1}	CMIPWRF
11	EDGARv5 (2015)		ED5WRF
12	EDGARv6.1 (2018)		ED6WRF
13	EDGAR-HTAPv3 (2018)		HTAPWRF
8	SMoG-COALESCCE (2019)		Nudged03
Nudging Strength and Approach Sensitivity Simulations			
14	Nudging Coeff. 0.0005 s^{-1}	ERA5 Meteorology, YSU PBL, Purdue Lin Microphysics, SMOG-COALESCCE Emission, MOZART – MOSAIC, Whole Atmosphere Nudging	Nudged05
15	Nudging Coeff. 0.001 s^{-1}		Nudged1
16	Nudging Coeff. 0.0003 s^{-1}	ERA5 Meteorology, YSU PBL, Purdue Lin Microphysics, SMOG-COALESCCE Emission, MOZART – MOSAIC, No Nudging within the PBL	NoNudPBL03
17	Nudging Coeff. 0.0005 s^{-1}		NoNudPBL05
18	Nudging Coeff. 0.001 s^{-1}		NoNudPBL1

Δ Surface Relative Humidity (%)

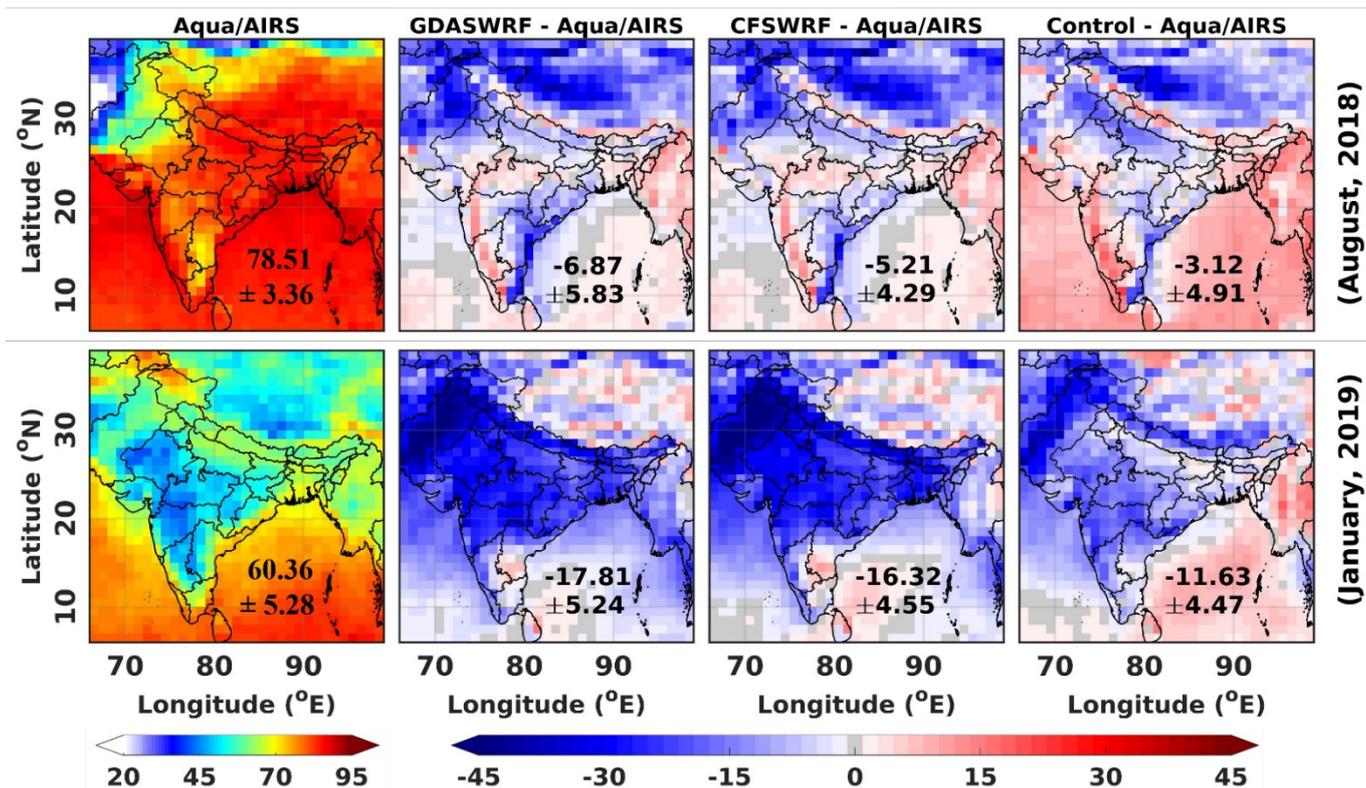


Figure S2. Spatial distribution of surface relative humidity observed by Aqua/AIRS over the Indian region, and the corresponding differences from various WRF-Chem meteorology sensitivity simulations. Inset values report the domain-mean \pm spatial standard deviation ($\mu \pm 1\sigma$) computed over the Indian landmass, along with Mean Bias Error (MBE) relative to Aqua/AIRS.

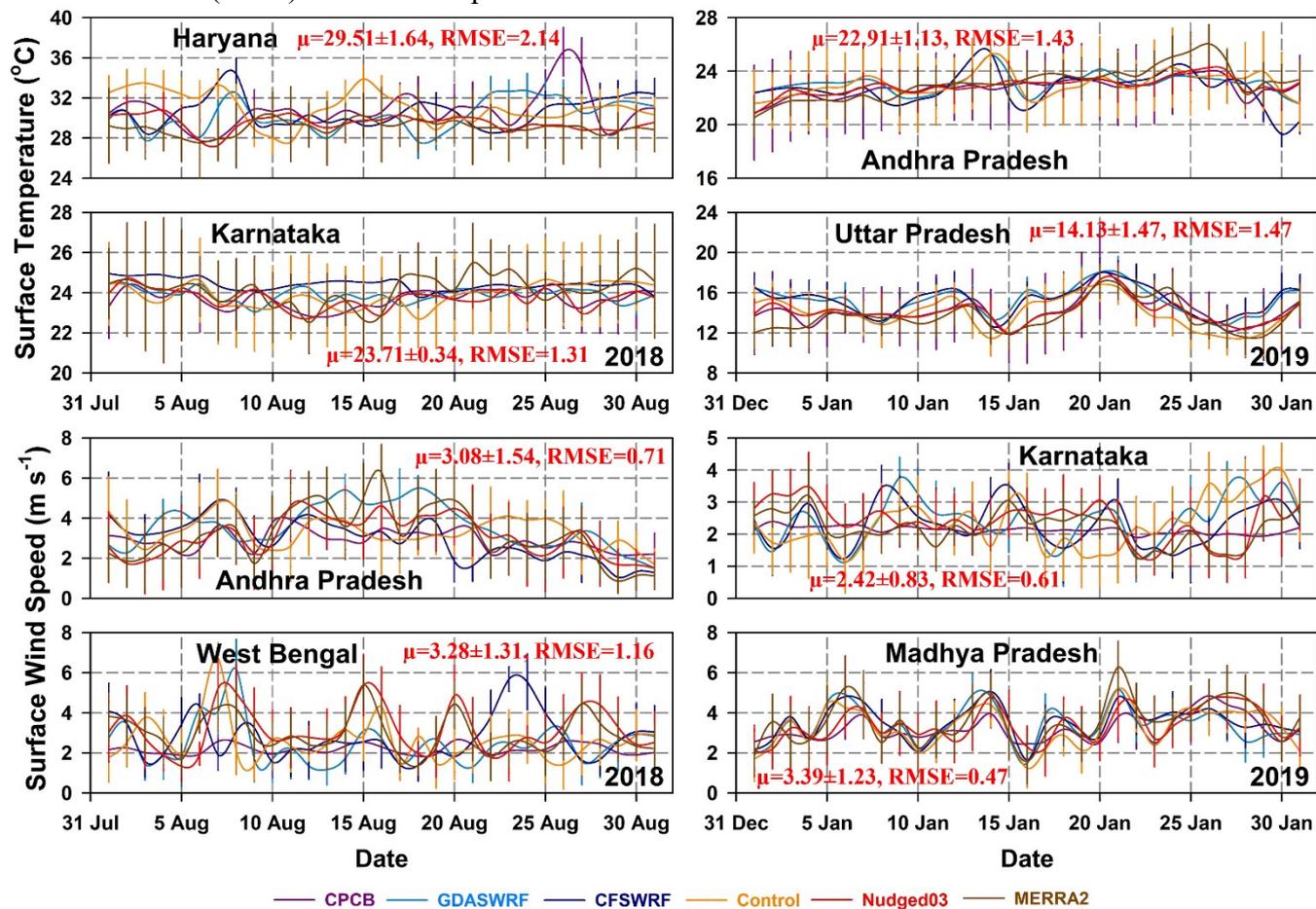


Figure S3. Daily mean time series comparison of surface temperature and surface wind speed for selected Indian states from different WRF-Chem meteorology and grid-nudging sensitivity simulations against CPCB measurements and MERRA2 reanalysis. Temporal mean \pm standard deviation ($\mu \pm 1\sigma$), together with correlation coefficient (r) and RMSE of Nudged03, are indicated within each panel.

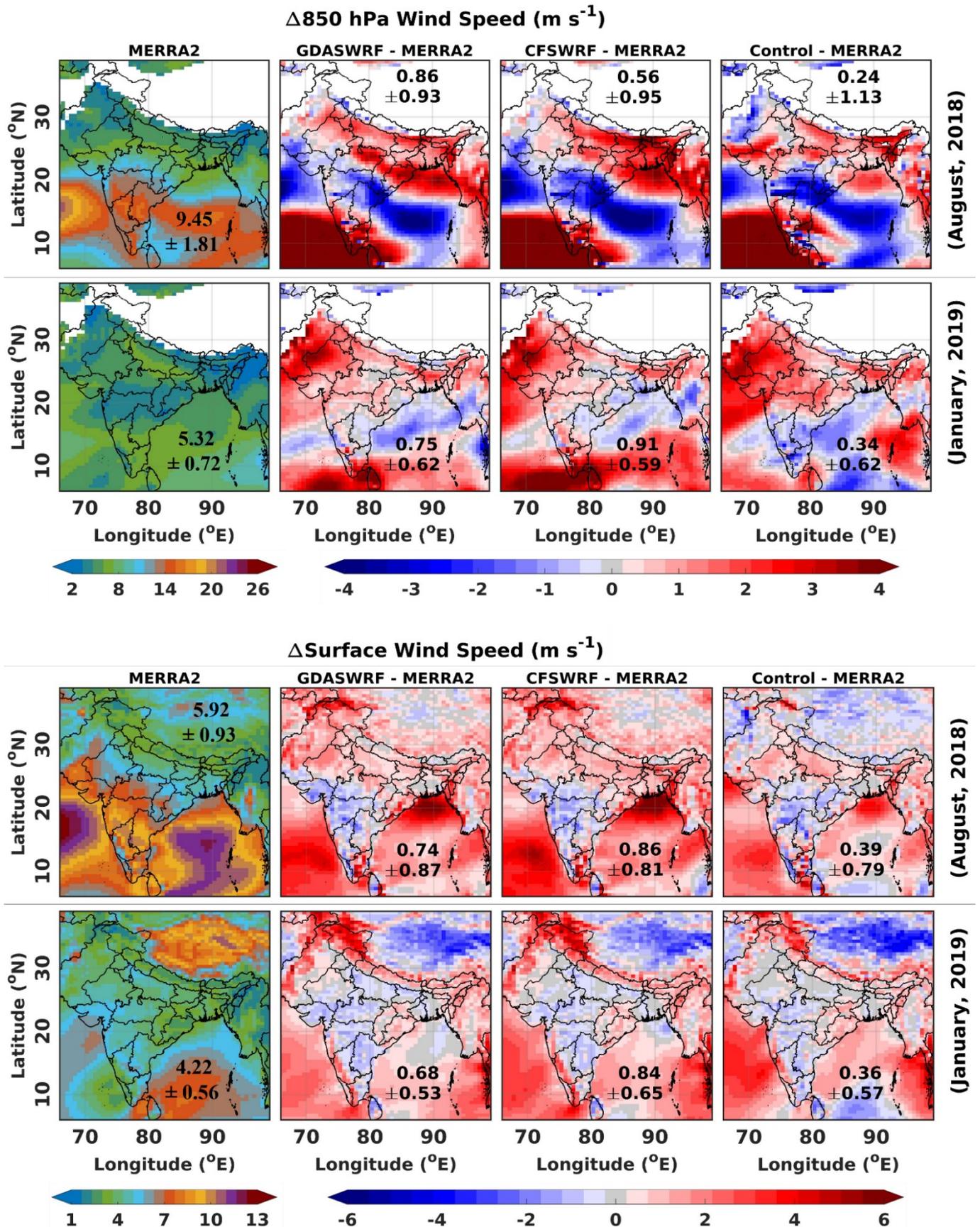


Figure S4. Spatial distribution of 850 hPa (top panel) and surface (bottom panel) wind speed from MERRA2 reanalysis over the Indian region and corresponding differences from various WRF-Chem meteorology sensitivity simulations. Inset values show domain-mean \pm spatial SD ($\mu \pm 1\sigma$) and Mean Bias Error (MBE) computed over the Indian landmass.

Table S2. Regression statistics for various meteorological variables over the Indian region from different meteorological and PBL sensitivity simulations for both study periods, evaluated against Aqua/AIRS and MERRA-2 observational datasets.

Regression Statistics for Surface Temperature between Aqua/AIRS and Different Meteorology Sensitivity Simulations										
		Control			GDASWRF			CFSWRF		
Common Model Configurations		YSU PBL, Purdue Lin Microphysics, SMOG-COALESCE Emission, MOZART – MOSAIC, No Nudging								
Month	Count	MBE	r	RMSE	MBE	r	RMSE	MBE	r	RMSE
August 2018	2812	0.87 (°C)	0.97	2.09 (°C)	1.17 (°C)	0.91	2.63 (°C)	1.13 (°C)	0.89	2.81 (°C)
January 2019	3811	-1.01 (°C)	0.96	2.39 (°C)	-1.65 (°C)	0.87	2.53 (°C)	-1.52 (°C)	0.88	2.43 (°C)
Regression Statistics for Surface Relative Humidity between Aqua/AIRS and Diff. Meteorology Sensitivity Simulations										
August 2018	2882	-3.12 (%)	0.49	14.72 (%)	-6.87 (%)	0.54	19.23 (%)	-5.21 (%)	0.58	17.76 (%)
January 2019	3943	-11.63 (%)	0.52	19.35 (%)	-17.81 (%)	0.56	23.26 (%)	-16.32 (%)	0.53	23.01 (%)
Regression Statistics for 850 hPa Wind Speed between MERRA2 and Different Meteorology Sensitivity Simulations										
August 2018	6217	0.24 (m s ⁻¹)	0.57	4.69 (m s ⁻¹)	0.86 (m s ⁻¹)	0.43	4.80 (m s ⁻¹)	0.56 (m s ⁻¹)	0.41	4.61 (m s ⁻¹)
January 2019	6217	0.34 (m s ⁻¹)	0.61	1.72 (m s ⁻¹)	0.75 (m s ⁻¹)	0.58	1.81 (m s ⁻¹)	0.91 (m s ⁻¹)	0.55	1.89 (m s ⁻¹)
Regression Statistics for Surface Wind Speed between MERRA2 and Different Meteorology Sensitivity Simulations										
August 2018	7936	0.39 (m s ⁻¹)	0.61	2.51 (m s ⁻¹)	0.74 (m s ⁻¹)	0.56	2.47 (m s ⁻¹)	0.86 (m s ⁻¹)	0.53	2.44 (m s ⁻¹)
January 2019	7936	0.36 (m s ⁻¹)	0.59	1.37 (m s ⁻¹)	0.68 (m s ⁻¹)	0.54	1.58 (m s ⁻¹)	0.84 (m s ⁻¹)	0.52	1.64 (m s ⁻¹)
Regression Statistics for PBL height between MERRA2 and Different PBL Sensitivity Simulations										
		Control			MYNWRF			MYJWRF		
August 2018	7936	0.13 (km)	0.45	0.27 (km)	0.16 (km)	0.42	0.36 (km)	0.17 (km)	0.41	0.33 (km)
January 2019	7936	0.11 (km)	0.49	0.18 (km)	0.15 (km)	0.44	0.21 (km)	0.14 (km)	0.38	0.21 (km)
Regression Statistics for 850 hPa Temperature between Aqua/AIRS and Different PBL Sensitivity Simulations										
August 2018	2812	0.32 (°C)	0.58	2.58 (°C)	0.86 (°C)	0.51	3.19 (°C)	0.41 (°C)	0.52	3.29 (°C)
January 2019	3811	0.17 (°C)	0.61	3.07 (°C)	-1.72 (°C)	0.63	2.79 (°C)	-1.25 (°C)	0.69	2.40 (°C)

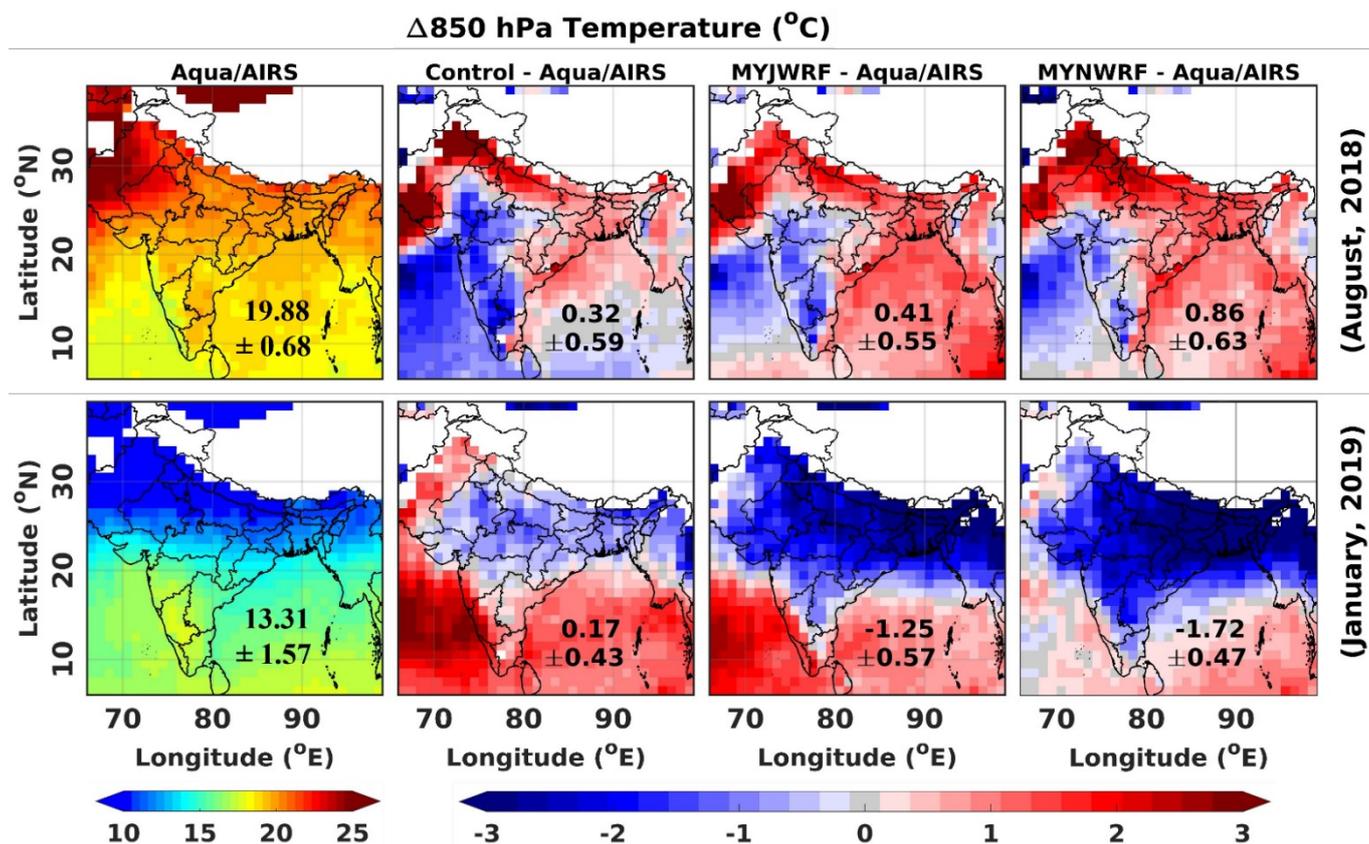


Figure S5. Spatial distribution of 850 hPa temperature observed by Aqua/AIRS over the Indian region, and the difference in simulated temperature from various WRF-Chem PBL sensitivity simulations. Domain-mean \pm spatial SD ($\mu \pm 1\sigma$) and Mean Bias Error (MBE) over the Indian landmass are reported within the panels.

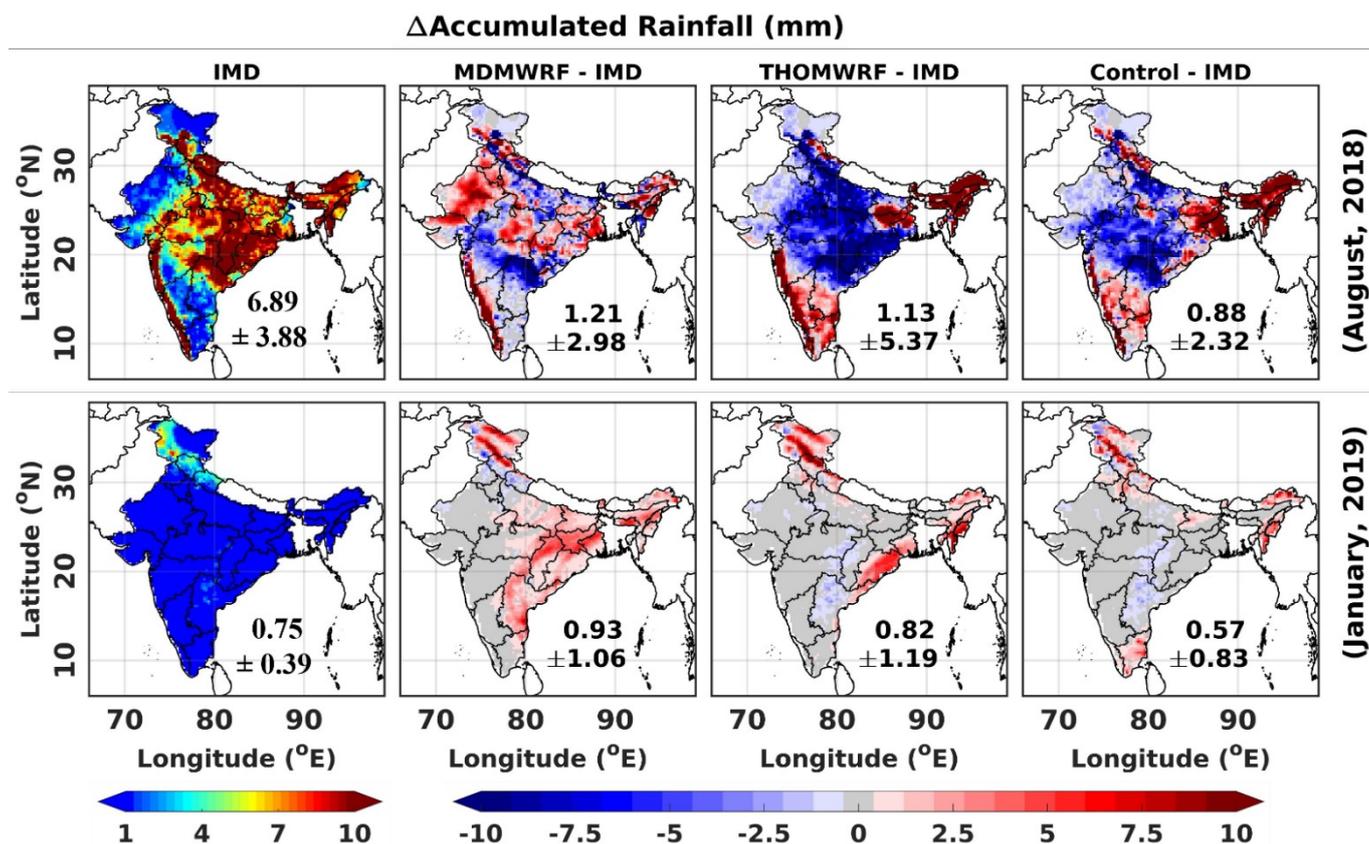


Figure S6. Spatial distribution of accumulated rainfall measured by the IMD over the Indian region and corresponding differences from various WRF-Chem microphysics sensitivity simulations. Inset statistics report domain-mean \pm spatial SD ($\mu \pm 1\sigma$) and Mean Bias Error (MBE) over the Indian landmass.

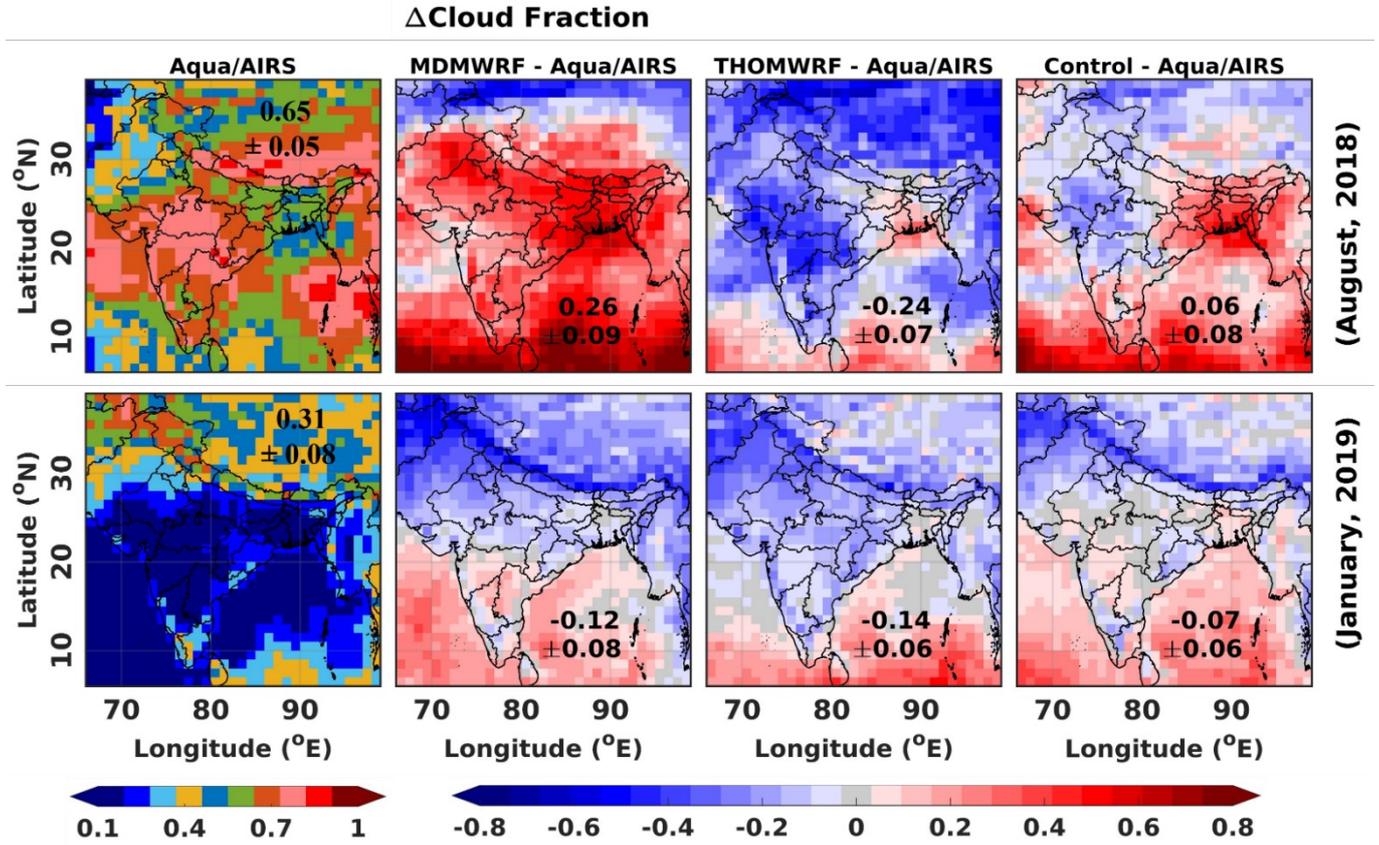


Figure S7. Spatial distribution of cloud fraction observed by Aqua/AIRS over the Indian region, and the difference in simulated cloud fraction from various WRF-Chem microphysics sensitivity simulations. Panels include domain-mean \pm spatial SD ($\mu \pm 1\sigma$) and Mean Bias Error (MBE) computed over the Indian landmass.

Table S3. Regression statistics for surface temperature, surface wind speed, surface relative humidity, cloud fraction and accumulated rainfall between various WRF-Chem microphysics sensitivity simulations with Aqua/AIRS observations, MERRA2 reanalysis, and IMD measurements over the Indian region for both study periods.

Regression Statistics for Surface Temperature between Aqua/AIRS and Different Microphysics Sensitivity Simulations										
		Control			THOMWRF			MDMWRF		
Common Model Configurations		ERA5 Meteorology, YSU PBL, SMOG-COALESCENCE Emission, MOZART – MOSAIC, No Nudging								
Month	Count	MAE	r	RMSE	MAE	r	RMSE	MAE	r	RMSE
August 2018	2812	1.20 (°C)	0.97	2.09 (°C)	3.03 (°C)	0.93	3.67 (°C)	1.77 (°C)	0.94	2.79 (°C)
January 2019	3811	1.72 (°C)	0.96	2.39 (°C)	2.77 (°C)	0.95	3.48 (°C)	2.84 (°C)	0.91	3.45 (°C)
Regression Statistics for Surface Temperature between MERRA2 and Different Microphysics Sensitivity Simulations										
August 2018	2812	1.36 (°C)	0.91	1.83 (°C)	2.48 (°C)	0.89	2.98 (°C)	1.75 (°C)	0.91	2.33 (°C)
January 2019	3811	2.11 (°C)	0.92	2.23 (°C)	2.37 (°C)	0.96	2.32 (°C)	2.41 (°C)	0.87	3.14 (°C)

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Regression Statistics for Surface Wind Speed between MERRA2 and Different Microphysics Sensitivity Simulations										
August 2018	7936	1.38 (m s ⁻¹)	0.61	2.51 (m s ⁻¹)	1.81 (m s ⁻¹)	0.61	2.38 (m s ⁻¹)	1.69 (m s ⁻¹)	0.63	2.17 (m s ⁻¹)
January 2019	7936	1.19 (m s ⁻¹)	0.59	1.37 (m s ⁻¹)	1.38 (m s ⁻¹)	0.58	1.89 (m s ⁻¹)	1.45 (m s ⁻¹)	0.39	1.98 (m s ⁻¹)
Regression Statistics for Surface Relative Humidity between Aqua/AIRS and Diff. Microphysics Sensitivity Simulations										
August 2018	2882	11.21 (%)	0.49	14.72 (%)	17.05 (%)	0.56	20.71 (%)	12.17 (%)	0.48	13.51 (%)
January 2019	3943	11.63 (%)	0.52	19.35 (%)	15.83 (%)	0.45	18.64 (%)	14.95 (%)	0.47	18.83 (%)
Regression Statistics for Accumulated Rainfall between IMD and Different Microphysics Sensitivity Simulations										
August 2018	3677	19.63 (mm)	0.37	12.16 (mm)	13.69 (mm)	0.34	18.55 (mm)	14.42 (mm)	0.33	16.28 (mm)
January 2019	307	7.36 (mm)	0.25	3.49 (mm)	6.68 (mm)	0.23	5.88 (mm)	6.71 (mm)	0.21	7.98 (mm)
Regression Statistics for Cloud Fraction between Aqua/AIRS and Different Microphysics Sensitivity Simulations										
August 2018	2882	1.16	0.63	0.21	1.78	0.57	0.29	2.62	0.54	0.37
January 2019	3943	2.14	0.59	0.17	1.68	0.54	0.25	1.41	0.52	0.21

Δ 850 hPa Ozone Concentration (O_3 , $\mu g m^{-3}$)

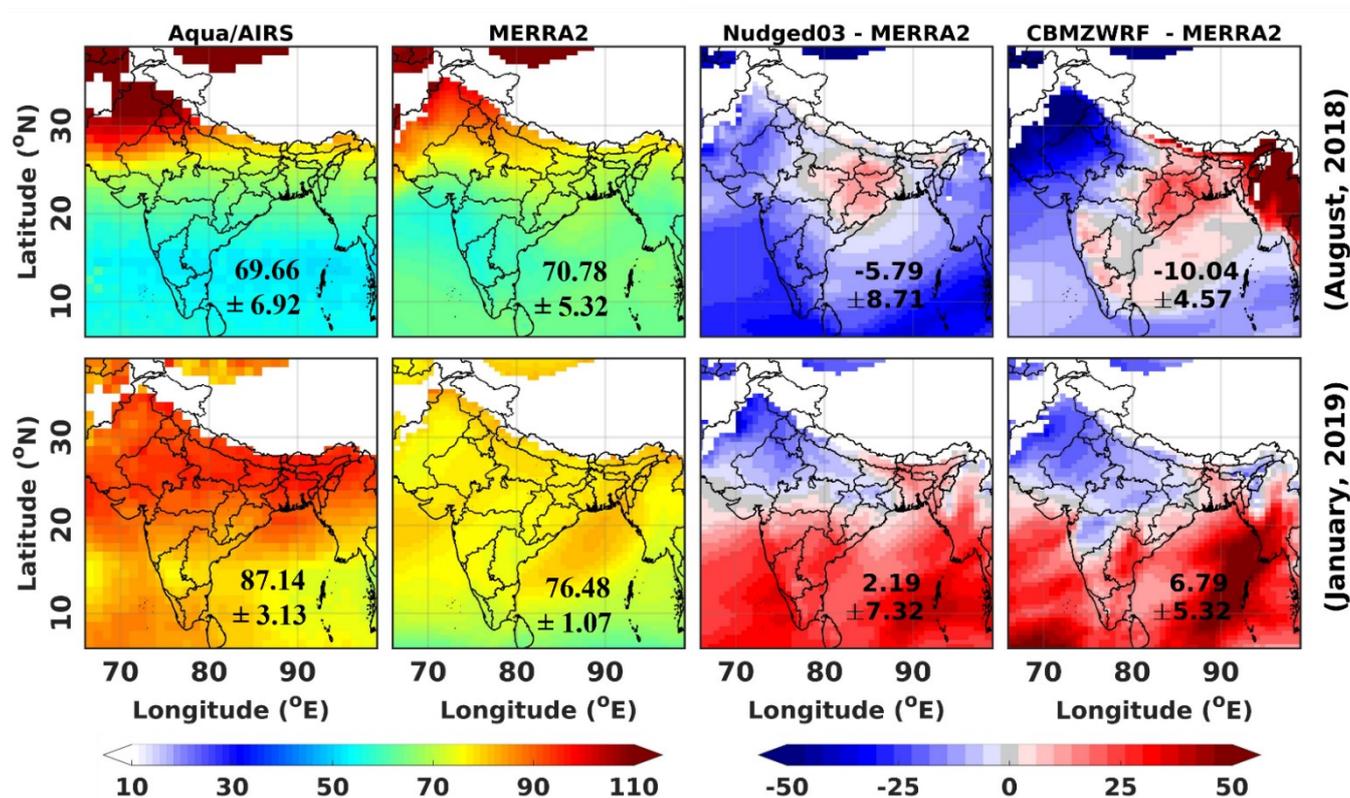


Figure S8. Spatial distribution of 850 hPa O_3 distribution observed by Aqua/AIRS, MERRA2 and the difference in simulated 850 hPa O_3 from different WRF-Chem chemical mechanism sensitivity simulations. Inset values show domain-mean \pm spatial SD ($\mu \pm 1\sigma$) and Mean Bias Error (MBE) relative to observations.

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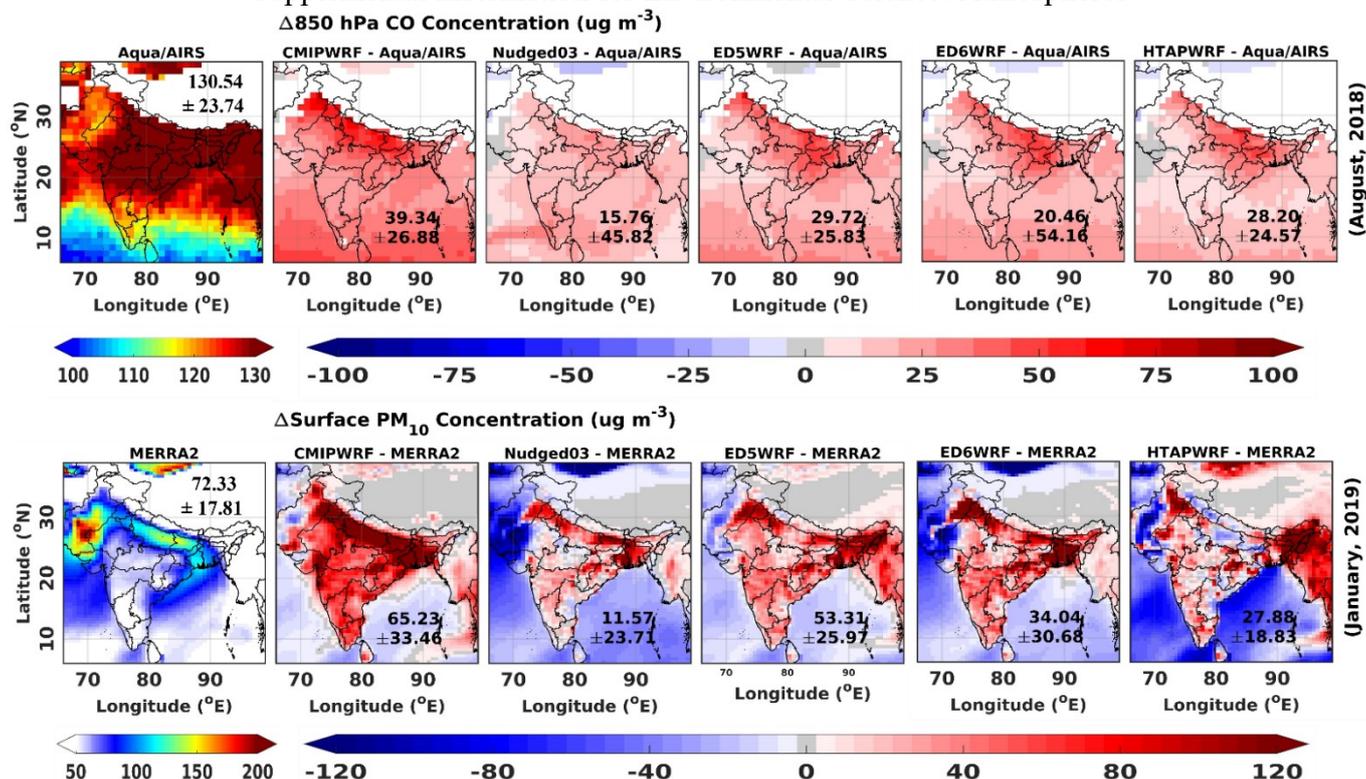


Figure S9. Spatial distribution of 850 hPa CO concentration by Aqua/AIRS over the Indian region, and the difference in simulated 850 hPa CO from various WRF-Chem emission inventory sensitivity simulations (top panel). Spatial distribution of surface PM_{10} concentration by MERRA2 over the Indian region, and the difference in simulated surface PM_{10} from various WRF-Chem emission inventory sensitivity simulations (bottom panel). For both panels, domain-mean \pm spatial SD ($\mu \pm 1\sigma$) and Mean Bias Error (MBE) over the Indian landmass are reported within the plots.

Table S4. Regression statistics for AOD, Surface $\text{PM}_{2.5}$, Surface PM_{10} and 850 hPa CO over the Indian region from different WRF-Chem Emission Inventory sensitivity simulations for both study periods, evaluated against Aqua/AIRS and MERRA-2 observational datasets.

Regression Statistics for AOD between MERRA2 and Different Emission Inventory Sensitivity Simulations																
		CMIPWRF			ED5WRF			ED6WRF			HTAPWRF			Nudged03		
Common Model Configurations		ERA5 Meteorology, YSU PBL, Purdue Lin Microphysics, MOZART – MOSAIC, Whole Atmosphere Nudging, Nudging Coeff. 0.0003 s^{-1}														
Month	Count	MBE	r	RMSE	MBE	r	RMSE	MBE	r	RMSE	MBE	r	RMSE	MBE	r	RMSE
August 2018	7936	0.13	0.47	0.39	0.24	0.51	0.40	0.10	0.48	0.26	0.45	0.32	0.62	0.07	0.56	0.27
January 2019	7936	-0.15	0.76	0.17	-0.14	0.74	0.18	-0.16	0.77	0.19	-0.19	0.72	0.22	-0.06	0.83	0.12
Regression Statistics for Surface $\text{PM}_{2.5}$ between MERRA2 and Different Emission Inventory Sensitivity Simulations																
August 2018	7936	45.21 $\mu\text{g/m}^3$	0.63	68.46 $\mu\text{g/m}^3$	32.29 $\mu\text{g/m}^3$	0.65	38.07 $\mu\text{g/m}^3$	13.24 $\mu\text{g/m}^3$	0.61	35.55 $\mu\text{g/m}^3$	40.51 $\mu\text{g/m}^3$	0.56	44.91 $\mu\text{g/m}^3$	8.56 $\mu\text{g/m}^3$	0.68	26.76 $\mu\text{g/m}^3$
January 2019	7936	64.08 $\mu\text{g/m}^3$	0.79	140.21 $\mu\text{g/m}^3$	59.38 $\mu\text{g/m}^3$	0.57	107.97 $\mu\text{g/m}^3$	29.81 $\mu\text{g/m}^3$	0.80	66.62 $\mu\text{g/m}^3$	32.60 $\mu\text{g/m}^3$	0.41	68.29 $\mu\text{g/m}^3$	16.52 $\mu\text{g/m}^3$	0.87	44.46 $\mu\text{g/m}^3$
Regression Statistics for Surface PM_{10} between MERRA2 and Different Emission Inventory Sensitivity Simulations																
August 2018	7936	32.66 $\mu\text{g/m}^3$	0.62	79.63 $\mu\text{g/m}^3$	25.10 $\mu\text{g/m}^3$	0.65	51.99 $\mu\text{g/m}^3$	23.74 $\mu\text{g/m}^3$	0.69	109.17 $\mu\text{g/m}^3$	21.09 $\mu\text{g/m}^3$	0.57	48.53 $\mu\text{g/m}^3$	17.34 $\mu\text{g/m}^3$	0.71	46.22 $\mu\text{g/m}^3$
January 2019	7936	65.23 $\mu\text{g/m}^3$	0.68	92.98 $\mu\text{g/m}^3$	53.31 $\mu\text{g/m}^3$	0.66	66.97 $\mu\text{g/m}^3$	34.04 $\mu\text{g/m}^3$	0.62	64.19 $\mu\text{g/m}^3$	27.88 $\mu\text{g/m}^3$	0.59	51.29 $\mu\text{g/m}^3$	11.57 $\mu\text{g/m}^3$	0.77	34.68 $\mu\text{g/m}^3$
Regression Statistics for 850 hPa CO between Aqua/AIRS and Different Emission Inventory Sensitivity Simulations																
August 2018	2812	39.34 $\mu\text{g/m}^3$	0.43	72.60 $\mu\text{g/m}^3$	29.72 $\mu\text{g/m}^3$	0.52	53.57 $\mu\text{g/m}^3$	20.46 $\mu\text{g/m}^3$	0.47	51.38 $\mu\text{g/m}^3$	28.20 $\mu\text{g/m}^3$	0.56	57.54 $\mu\text{g/m}^3$	15.76 $\mu\text{g/m}^3$	0.63	44.75 $\mu\text{g/m}^3$
January 2019	3811	35.52 $\mu\text{g/m}^3$	0.51	84.40 $\mu\text{g/m}^3$	29.28 $\mu\text{g/m}^3$	0.53	105.96 $\mu\text{g/m}^3$	22.82 $\mu\text{g/m}^3$	0.49	54.92 $\mu\text{g/m}^3$	27.11 $\mu\text{g/m}^3$	0.55	60.91 $\mu\text{g/m}^3$	15.54 $\mu\text{g/m}^3$	0.61	36.82 $\mu\text{g/m}^3$

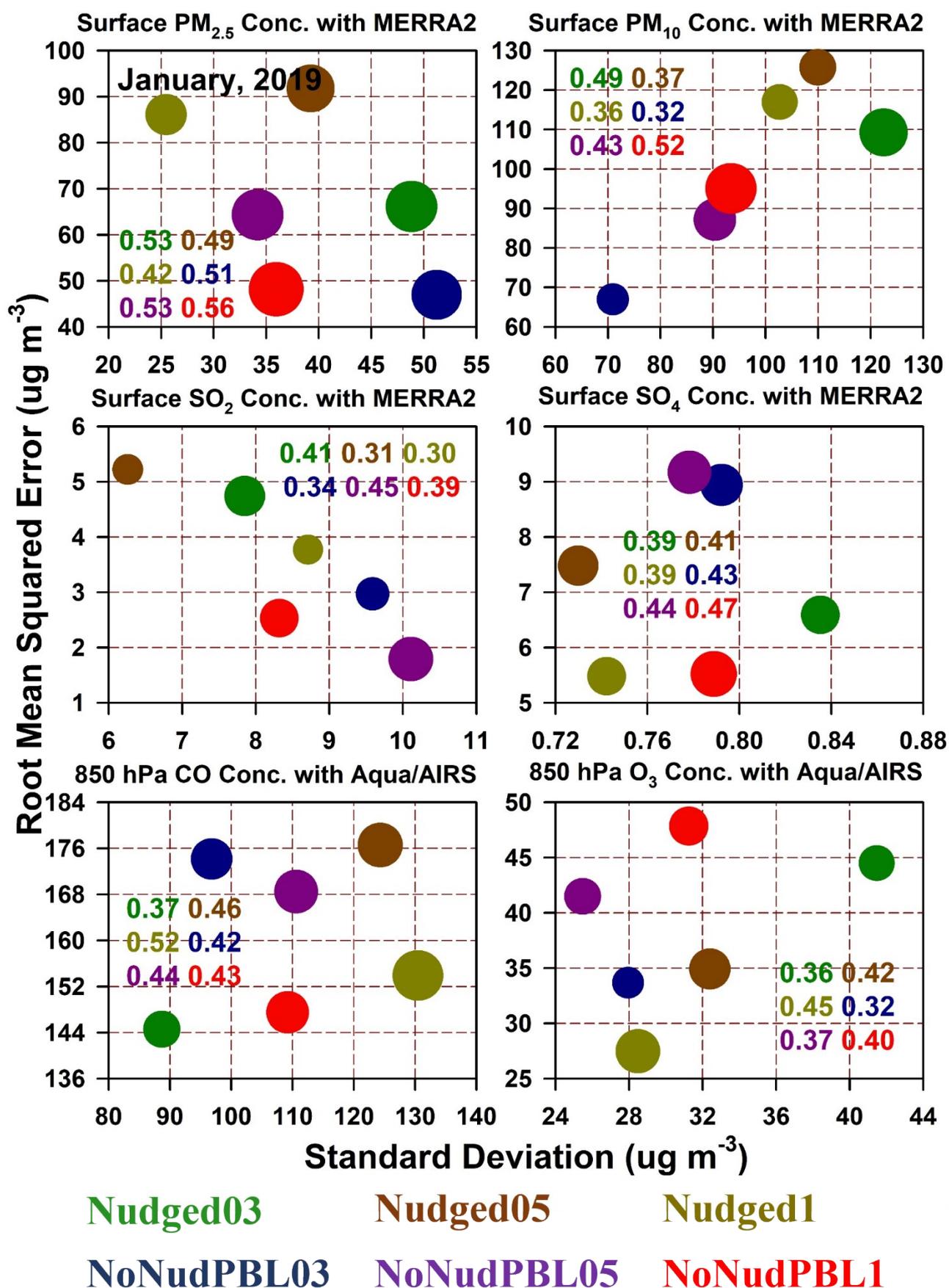


Figure S10. Bubble plot representation of statistical comparisons for various surface and 850 hPa pollutants over the Indian region against MERRA2 and Aqua/AIRS for different WRF-Chem nudging coefficient

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 sensitivity simulations for January 2019. Bubble size represents RMSE, colour indicates various experiments, and inset values show Coefficients of determination (r^2).

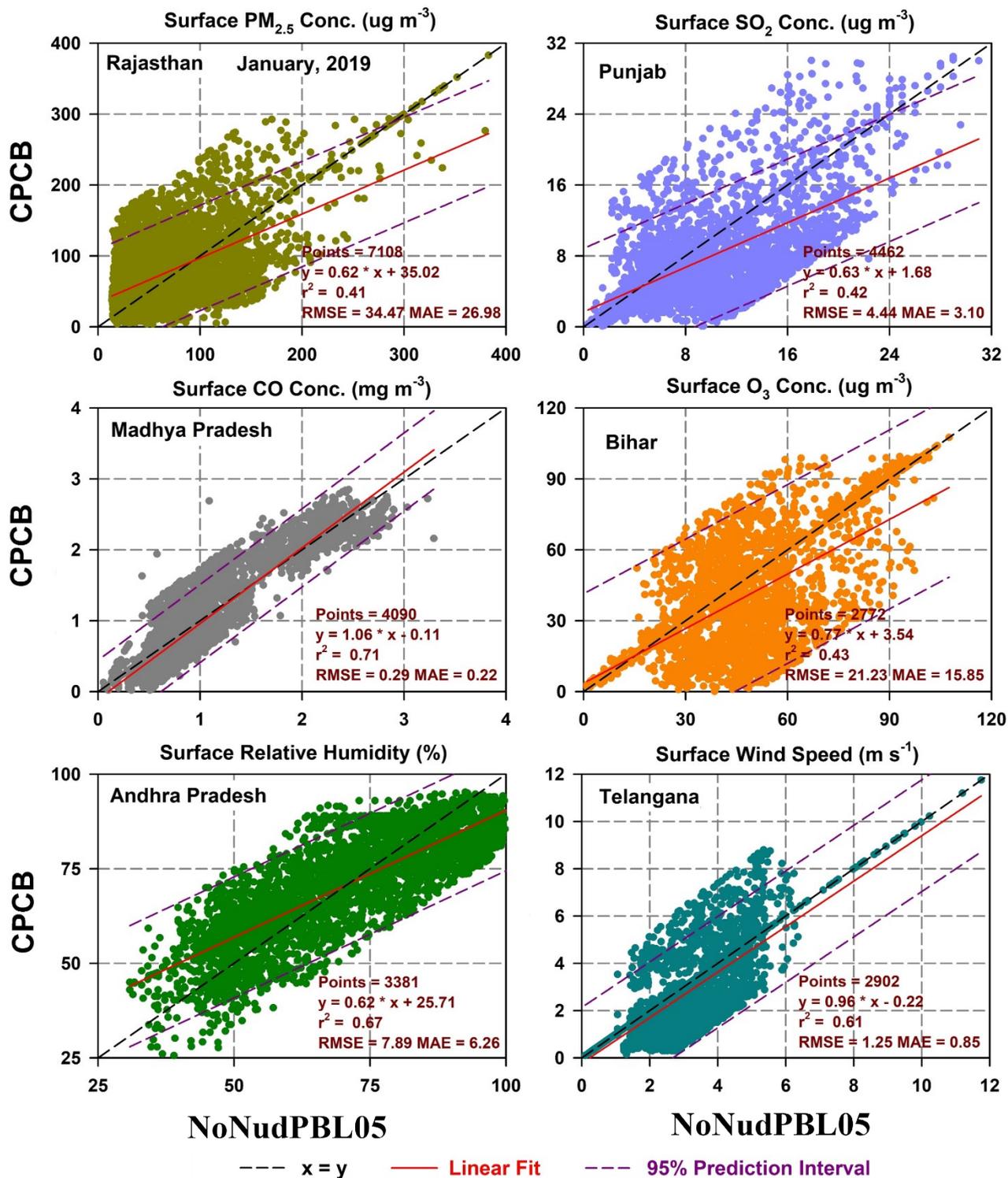


Figure S11. A statistical comparison of preferred WRF-Chem-simulated meteorological parameters and pollutant concentrations with CPCB measurements is shown for various Indian states with available continuous monitoring data (see Figure S1) for January 2019. Panels report state-wise regression statistics (MAE, RMSE, and r^2) indicated in parentheses, enabling direct quantitative assessment of model skill across regions.

Table S5. Regression statistics Surface PM_{2.5}, PM₁₀, SO₂ and SO₄ over the Entire Indian region from different WRF-Chem chemical mechanism, grid-nudging, grid-nudging strength and approach sensitivity simulations for both study periods, evaluated against MERRA-2 observational datasets.

Regression Statistics for Surface PM _{2.5} between MERRA2 and Different WRF-Chem Sensitivity Simulations Over India												
Month	Control			CBMZWF			Nudged03			Nudged05		
	MAE (ug/m ³)	r ²	RMSE (ug/m ³)	MAE (ug/m ³)	r ²	RMSE (ug/m ³)	MAE (ug/m ³)	r ²	RMSE (ug/m ³)	MAE (ug/m ³)	r ²	RMSE (ug/m ³)
August 2018	13.62	0.33	27.48	15.47	0.35	23.32	12.43	0.37	21.67	14.61	0.31	35.83
January 2019	28.47	0.48	69.74	32.48	0.51	70.15	34.18	0.53	66.14	27.45	0.49	91.75
Regression Statistics for Surface PM ₁₀ between MERRA2 and Different WRF-Chem Sensitivity Simulations Over India												
Month	Control			CBMZWF			Nudged03			Nudged05		
	MAE (ug/m ³)	r ²	RMSE (ug/m ³)	MAE (ug/m ³)	r ²	RMSE (ug/m ³)	MAE (ug/m ³)	r ²	RMSE (ug/m ³)	MAE (ug/m ³)	r ²	RMSE (ug/m ³)
August 2018	57.48	0.40	105.74	63.47	0.40	99.48	58.49	0.41	106.81	61.95	0.35	109.61
January 2019	73.47	0.45	111.78	88.47	0.46	103.24	85.73	0.49	109.25	76.94	0.37	125.73
Regression Statistics for Surface SO ₂ between MERRA2 and Different WRF-Chem Sensitivity Simulations Over India												
Month	Control			CBMZWF			Nudged03			Nudged05		
	MAE (ug/m ³)	r ²	RMSE (ug/m ³)	MAE (ug/m ³)	r ²	RMSE (ug/m ³)	MAE (ug/m ³)	r ²	RMSE (ug/m ³)	MAE (ug/m ³)	r ²	RMSE (ug/m ³)
August 2018	6.14	0.32	7.78	5.47	0.33	8.74	4.95	0.35	6.08	4.09	0.37	6.68
January 2019	6.89	0.39	6.93	6.73	0.38	5.88	5.51	0.41	4.74	4.38	0.31	5.22
Regression Statistics for Surface SO ₄ between MERRA2 and Different WRF-Chem Sensitivity Simulations Over India												
Month	Control			CBMZWF			Nudged03			Nudged05		
	MAE (ug/m ³)	r ²	RMSE (ug/m ³)	MAE (ug/m ³)	r ²	RMSE (ug/m ³)	MAE (ug/m ³)	r ²	RMSE (ug/m ³)	MAE (ug/m ³)	r ²	RMSE (ug/m ³)
August 2018	3.29	0.25	9.77	2.12	0.35	7.87	1.22	0.27	9.48	1.25	0.38	8.57
January 2019	3.78	0.36	6.83	3.47	0.45	8.74	1.51	0.39	6.59	1.31	0.41	7.48

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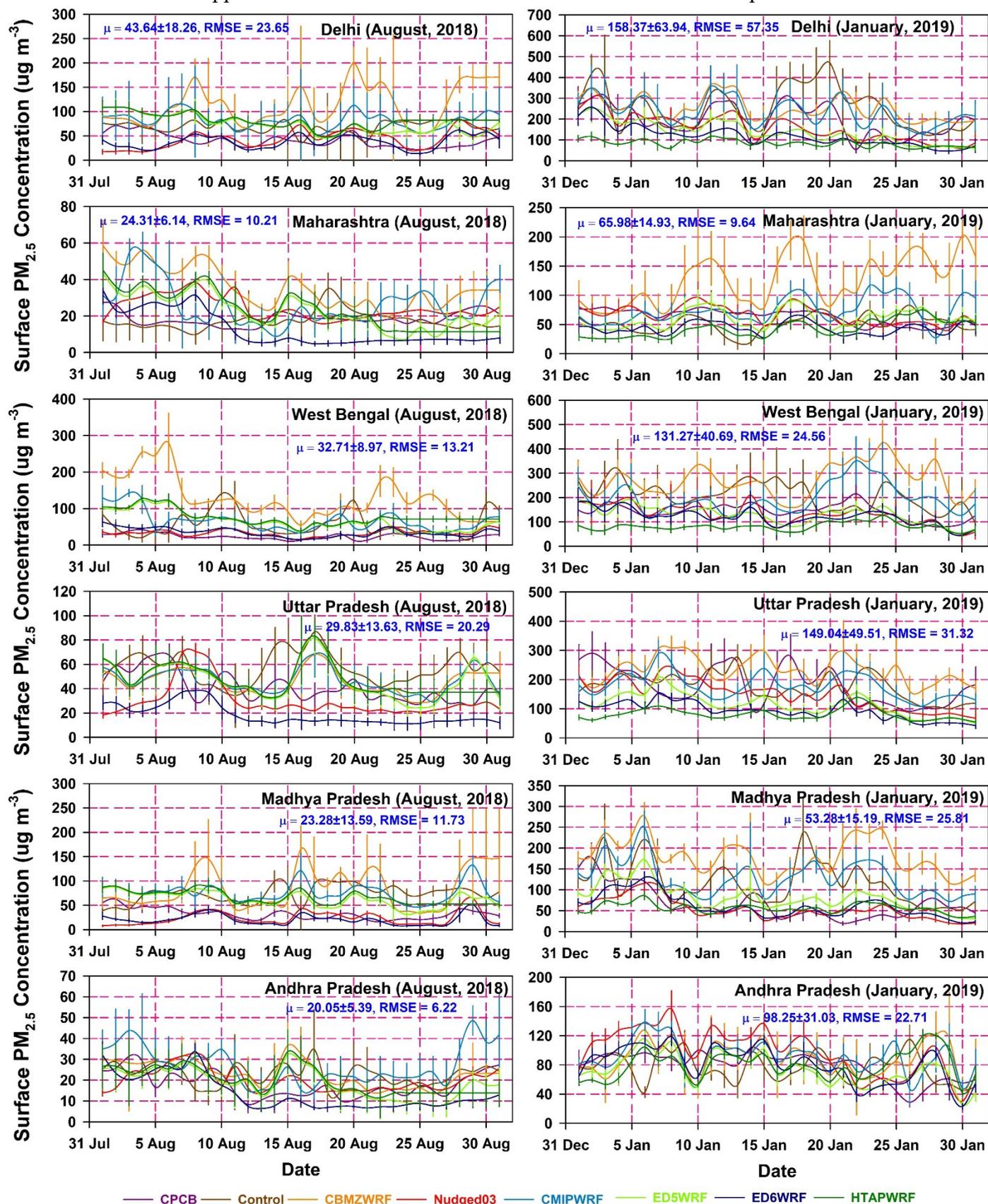


Figure S12. Daily mean time series comparison of surface $PM_{2.5}$ for selected Indian states from different WRF-Chem chemical mechanism and emission inventory sensitivity simulations against CPCB measurements. Temporal mean \pm standard deviation ($\mu \pm 1\sigma$), together with RMSE of Nudged03, are indicated within each panel.

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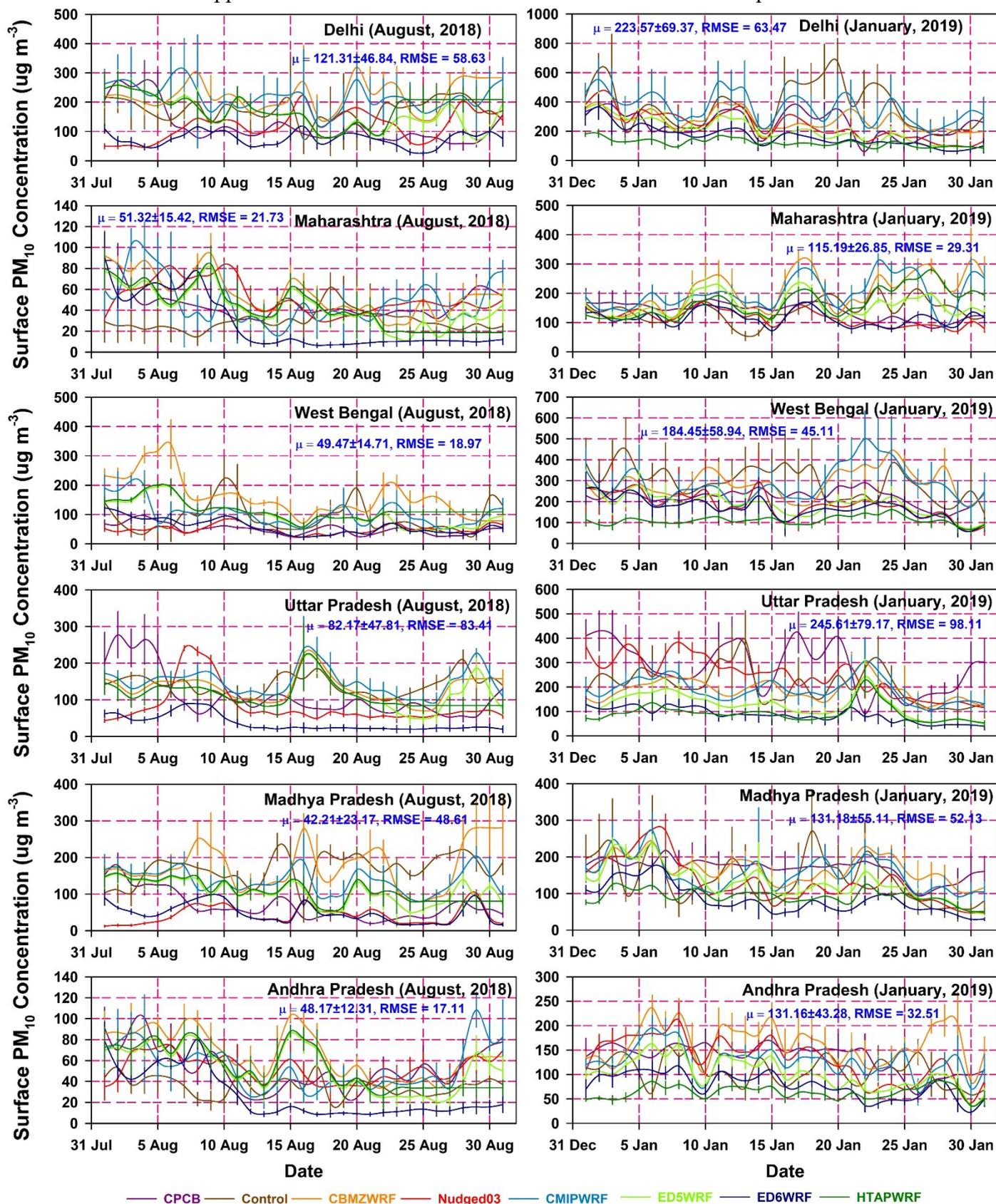


Figure S13. Daily mean time series comparison of surface PM_{10} for selected Indian states from different WRF-Chem chemical mechanism and emission inventory sensitivity simulations against CPCB measurements. Temporal mean \pm standard deviation ($\mu \pm \sigma$), together with RMSE of Nudged03, are indicated within each panel.

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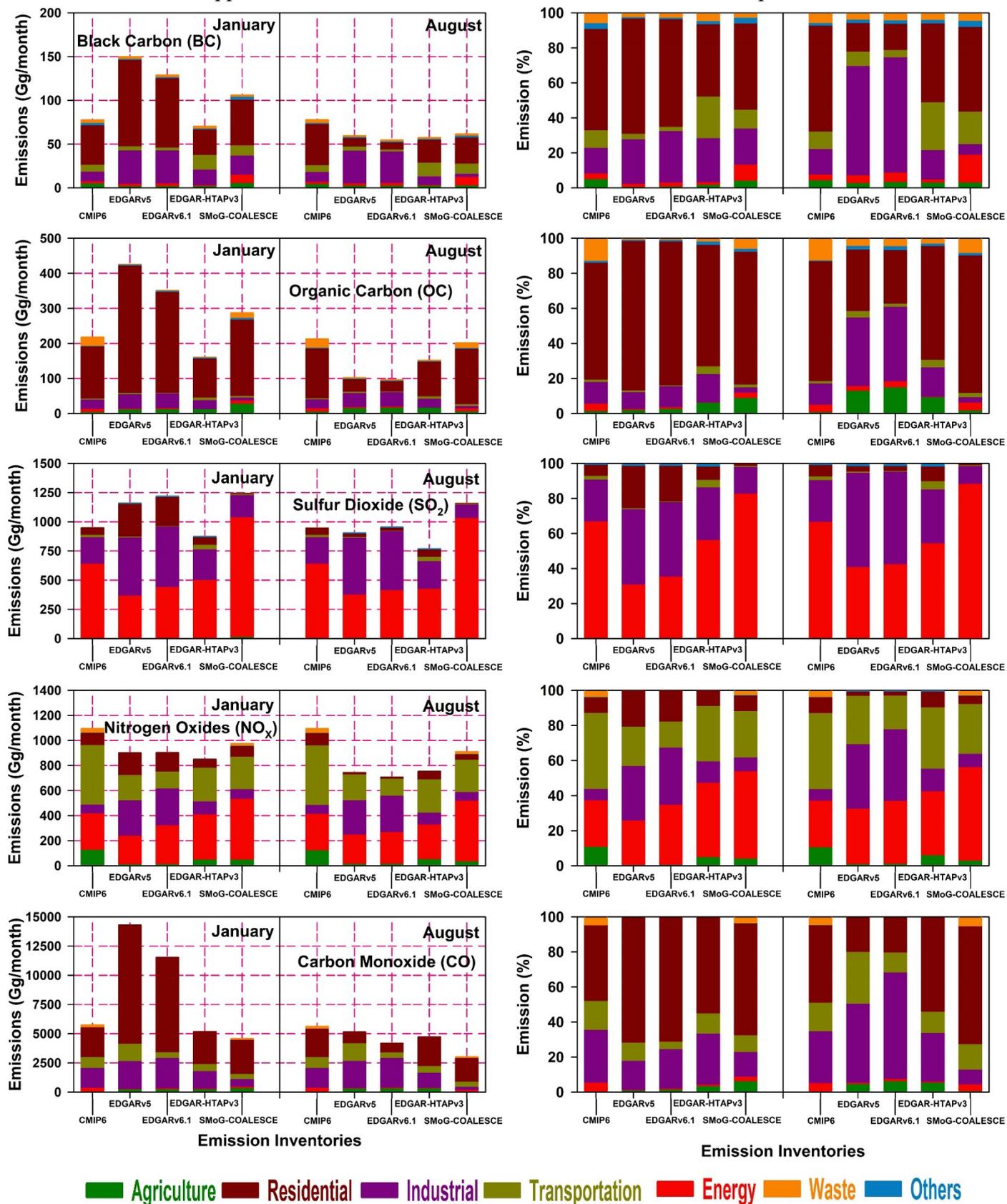


Figure S14. Bar charts showing the monthly total and sectoral emission comparison over India from different emission inventories used in the WRF-Chem emission inventory sensitivity simulations for various primary anthropogenic chemical species for August and January (left panel). The right panel represents the relative contribution of different emission sectors to the total emissions over the Indian region for the respective chemical species and period.