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Supporting Information for

Elucidating the Impacts of COVID-19 Lockdown on Air Quality and Ozone Chemical Characteristics in India

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Introduction

The supporting information includes an overview of comparison between the results using HTAP v2.2 and CAMS v4.2 emission inventories (Text S1), a guideline how to use the IRR outputs of WRF-Chem model (Text S2), and figures and tables supporting the results in the main manuscript.

Text S1- Comparing results using HTAP v2.2 and CAMS v4.2 anthropogenic emission inventories

To evaluate how changing anthropogenic emission inventories affect simulation results, we performed a set of experiments using HTAP v2.2 and the Copernicus Atmosphere Monitoring Service global emission inventory version 4.2 (CAMS v4.2) available from ECCAD database (https://permalink.aeris-data.fr/CAMS-GLOB-ANT, last access: 02/23/2021). CAMS v4.2 provides 0.1x0.1 degree gridded monthly-averaged emissions for the years between 2000 and 2020. It uses Emissions Database for Global Atmospheric Research version 4.3.2 (EDGARv4.3.2) for the years before 2012 and projects emissions between 2012 and 2020 using the Community Emissions Data System (CEDS) emission trends (Granier et al., 2019). Comparing CAMS v4.2 and HTAP v2.2 emissions for Delhi (i.e. Urban) indicated about 100% and 200% higher BC and OC emissions, respectively, in CAMS v4.2 inventory. CAMS v4.2 also showed higher CO (32%) emission, while lower NOx (23%) and SO2 (12%) emissions. NMVOC emissions was roughly similar in both inventories.

Statistics using CAMS v4.2 emission inventory were improved (Table S4-S5). In April 2019, the NMB for daily $PM_{2.5}$ and daytime ozone decreased by 10% and 12%, respectively. In April 2020, the NMB for daily $PM_{2.5}$ decreased by 47% and decreased by 10% for daytime ozone. Overall, the model performance using both emission inventories were within the benchmark criteria for daily $PM_{2.5}$ concentrations. Moreover, the performance for daytime ozone concentration was similar using both inventories Although there are some local emission inventories available throughout the country (Guttikunda et al., 2019;Jena et al., 2021), this experiment showed the necessity of an updated gridded national emission inventory for India. Regardless, our primary goal in this study was to investigate how the emission changes affected concentrations changes rather than capturing the actual concentrations. Results using CAMS emissions are very similar to those using HTAP as Figure S15 shows.

Text S2. Using IRR data in WRF-Chem model

IRR provides the gas-phase reaction rate for the species involved in each reaction. As a simple unit for these outputs, IRR within the WRF-Chem model, are in ppb and are cumulative. As a result, the hourly reaction rates (ppb/hr) can be calculated by subtracting the values in two consecutive hours. We use the difference between hours “i” and “i+1” as the reaction rate in hour “i”. Reporting this information in ‘ppb/hr’ makes the data easy-to-report and useful for all the species within the reaction. For example, in the reaction A+B-> C+D, a single reaction rate of RR in ppb/hr shows that RR ppb of A and B was consumed and RR ppb of C and D was produced in a specific hour. In our analysis, we used the IRR information averaged within the boundary layer following Pfister et al. (2019).

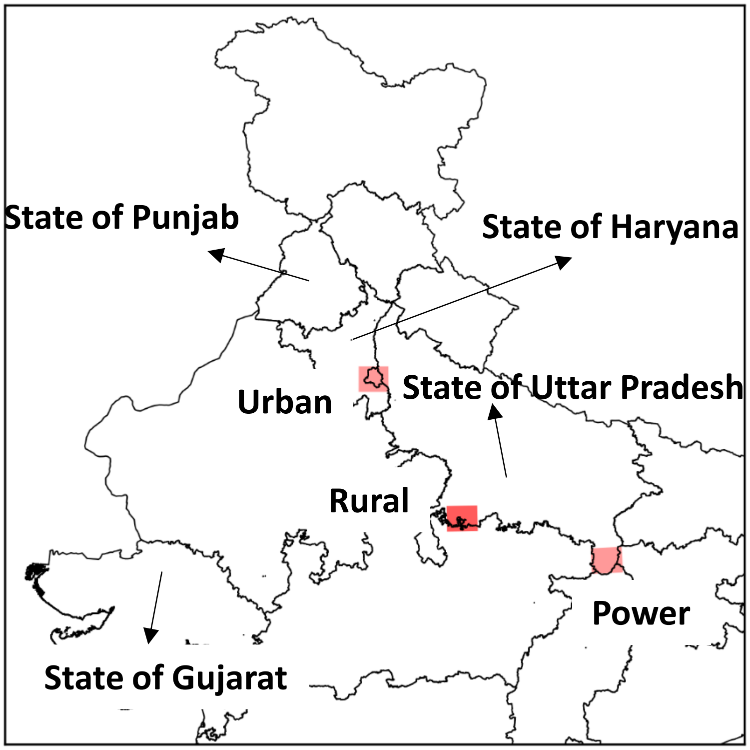

Figure S1 Location of the selected regions of Urban (Lower Left (LL): 28.3N, 76.7E, Upper Right (UR): 28.9N, 77.5E), Rural (LL: 25N, 79E, UR: 25.6N, 79.8E), and Power (LL: 23.9N, 82.7E, UR: 24.5N, 83.5E). States of Punjab, Haryana, Uttar Pradesh, and Gujarat are also shown.

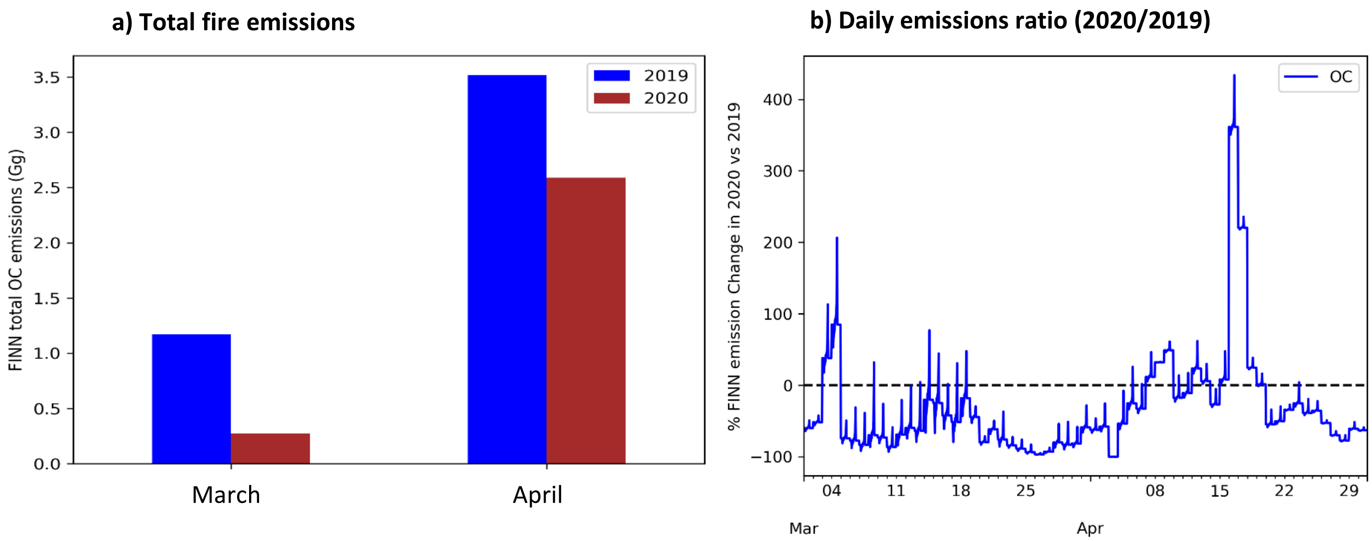

Figure S2 Comparison of FINN biomass burning emissions between 2019 and 2020 for a) total emissions and b) the ratio of daily emissions

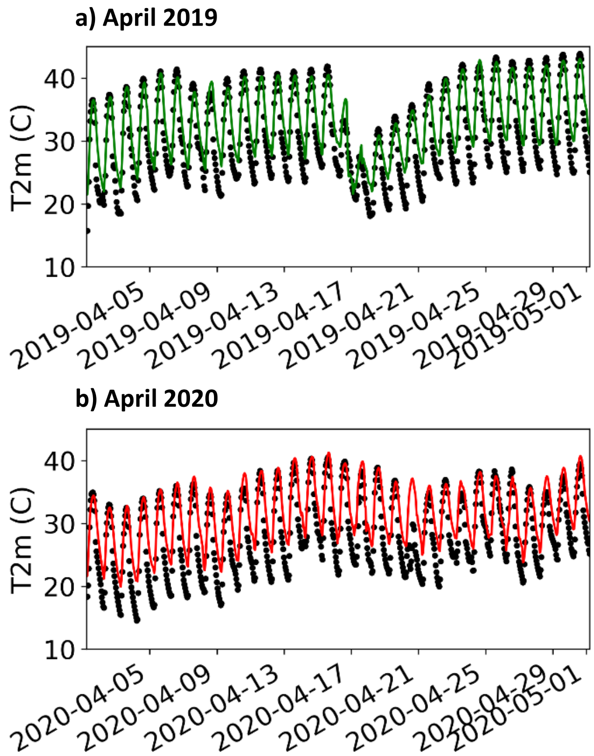

Figure S3 Timeseries of 2m temperature in model (black dots) and MERRA-2 (green line in 2019 (a) and red line in 2020 (b)) in a grid cell over Delhi (28.6N, 77.19 E)

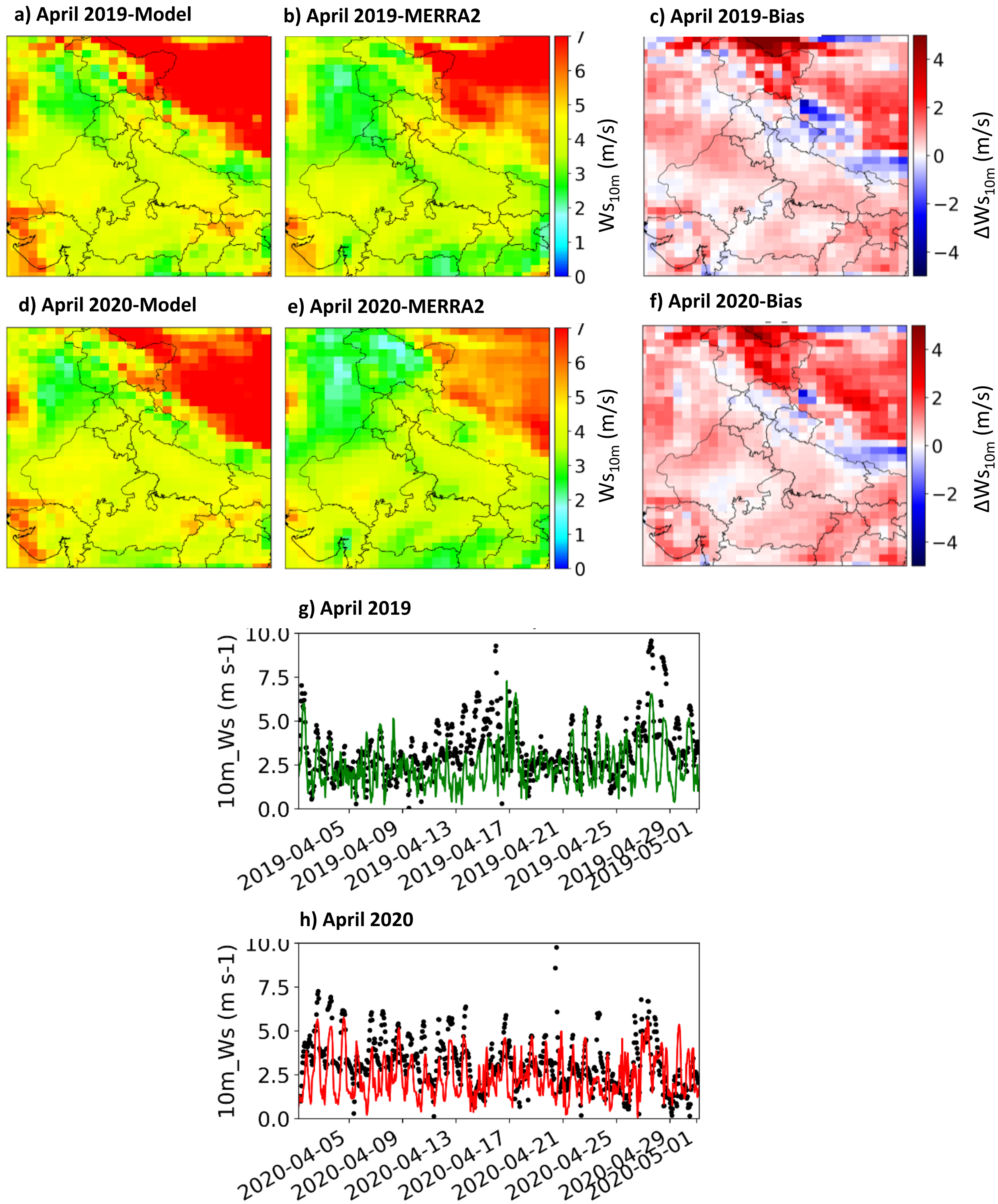

Figure S4 Temporospatial performance of the model for 10 m wind speed in April 2019 and 2020. Timeseries (g,h) are for a location in Delhi (28.6N, 77.19 E)

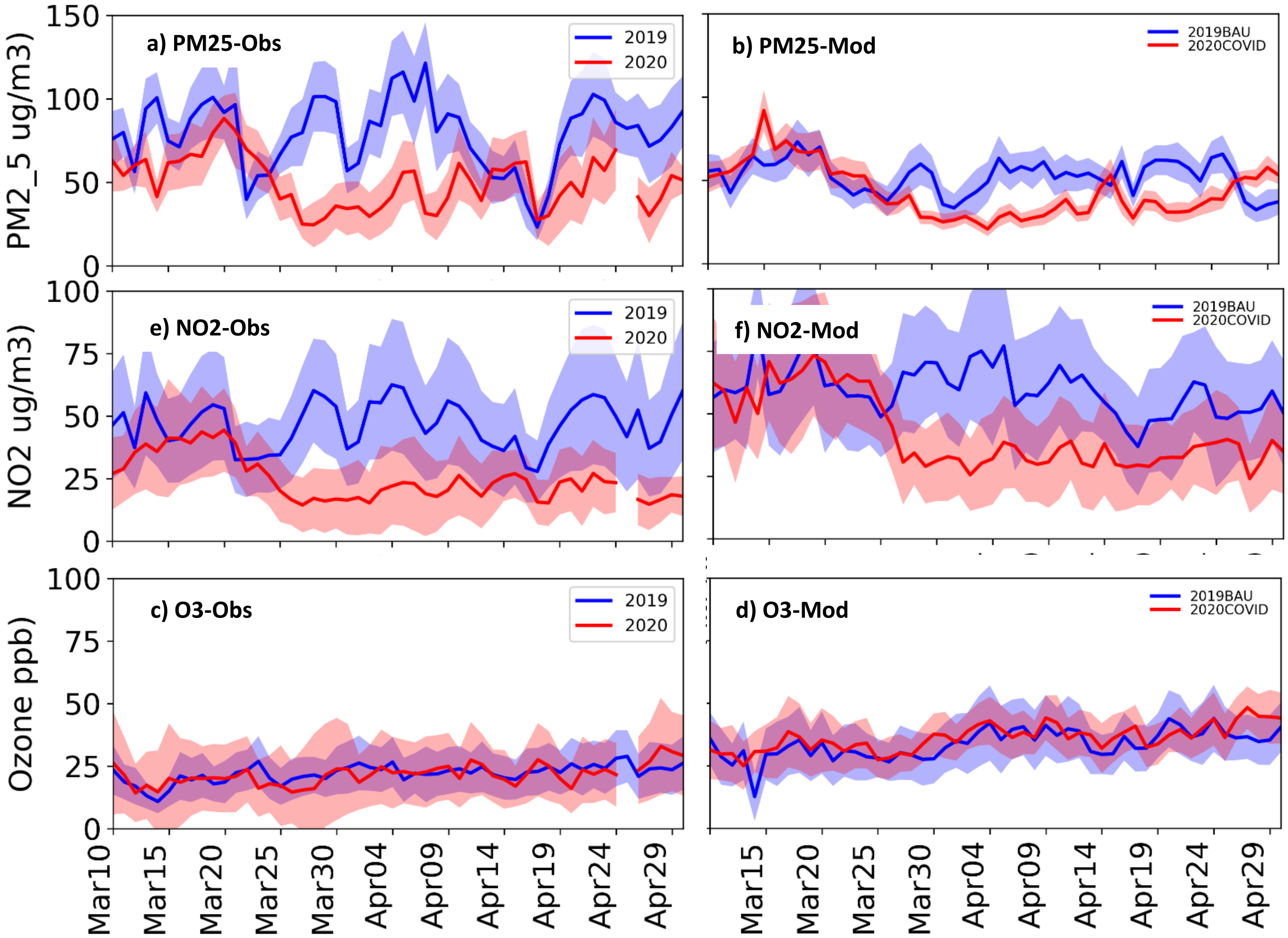

Figure S5 24-hour averaged $PM_{2.5}$ (top row), NO_2 (middle row), and ozone (bottom row) concentrations measured over CPCB stations in Delhi (left column) and modeled over Urban region (right column) between 10 March and 30 April in 2019 (green colors) and 2020 (red colors). The shaded regions show ±1STD. The observed data were extracted from the ground measurements data in Delhi, while the modeled data were averaged in the Urban subdomain.

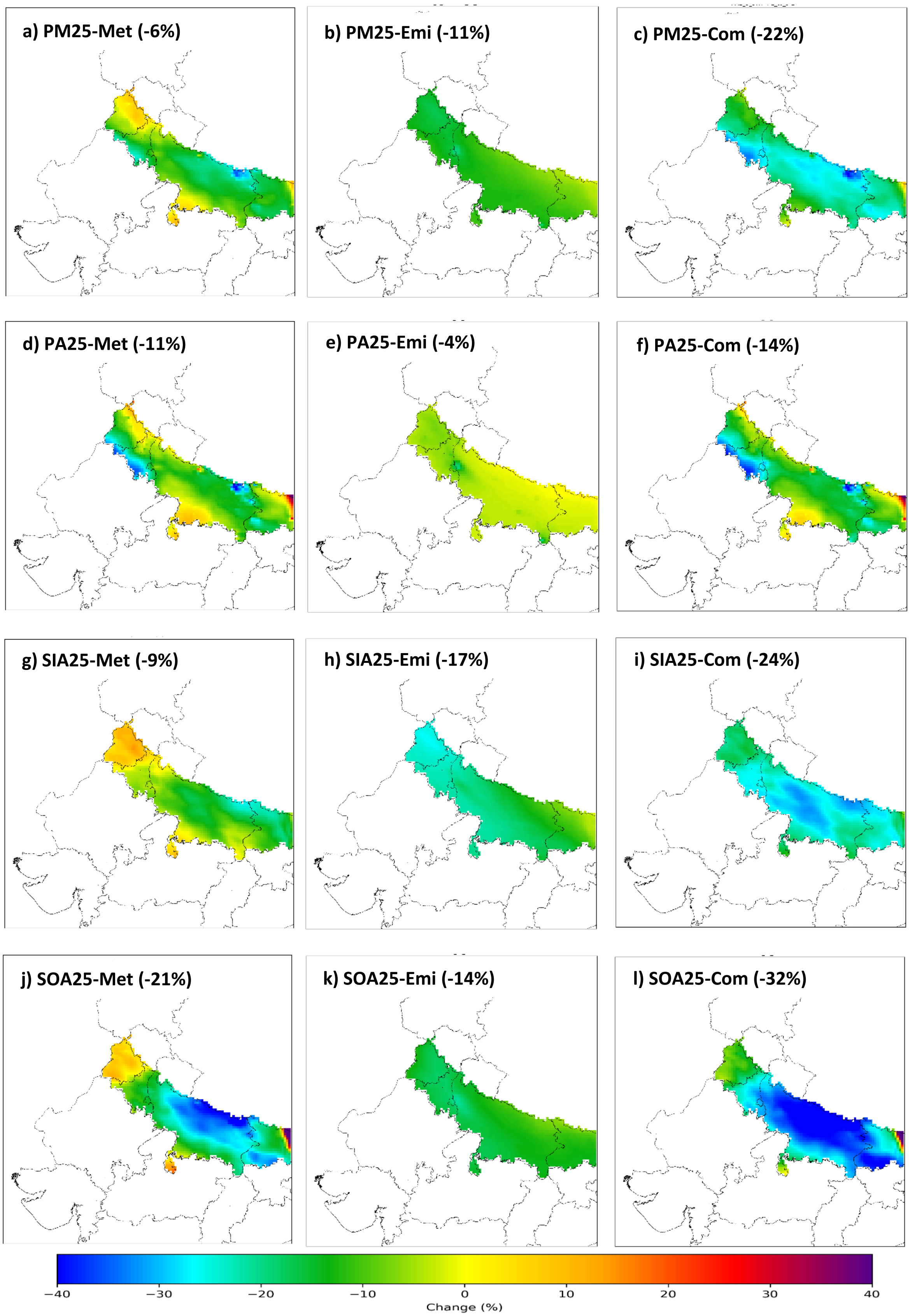

Figure S6 Responses of April averaged daytime $PM_{2.5}$ (first row), $PA_{2.5}$ (second row), $SIA_{2.5}$ (third row), and $SOA_{2.5}$ (fourth row) concentrations in the IGP to meteorology (left column), emission (middle column), and combined (right column) effects. The numbers in the parenthesis show the averaged change over the colored region between April 2020 and 2019.

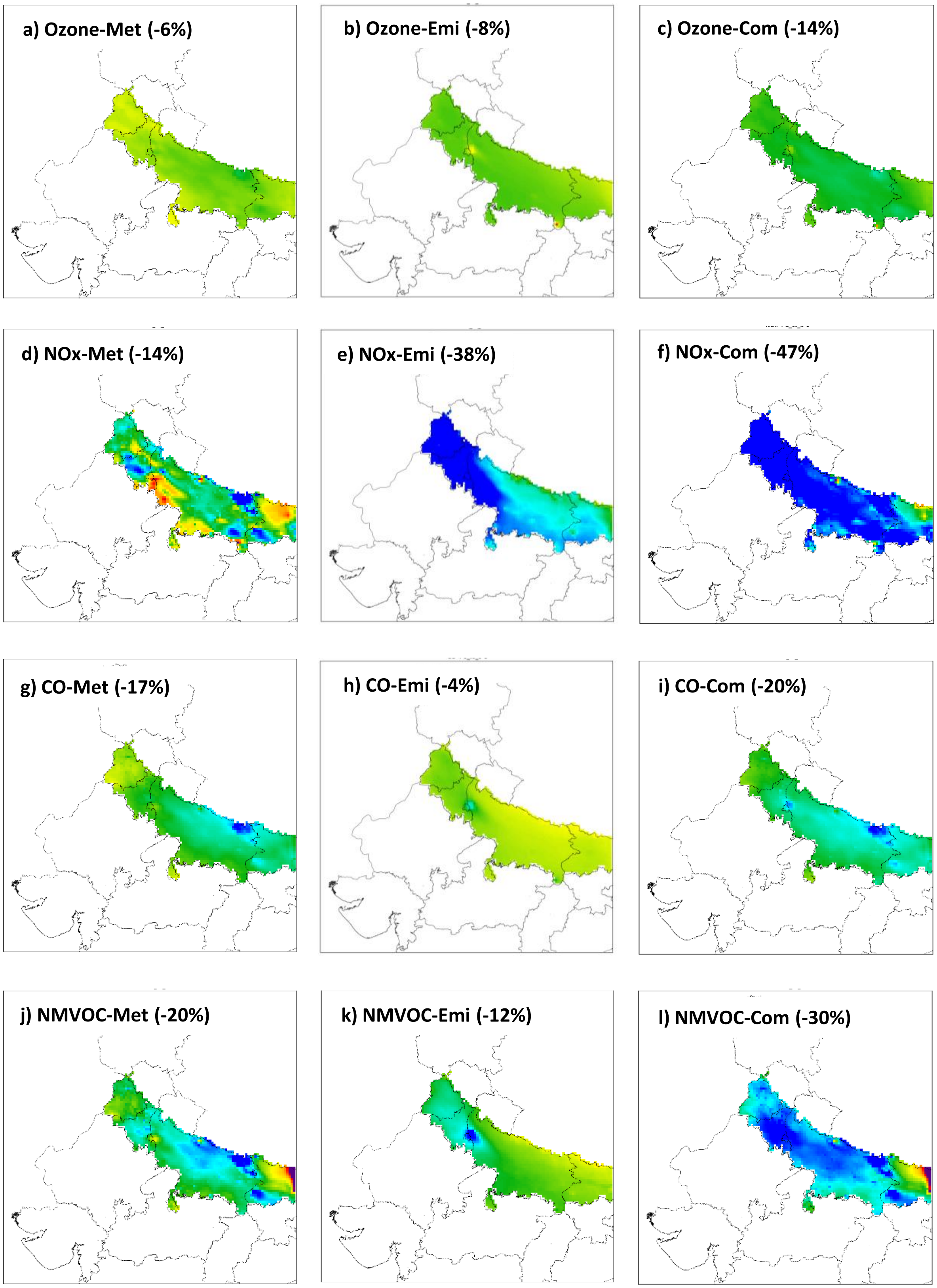

Figure S7 Responses of April averaged daytime ozone (first row), NOx (second row), CO (third row), and NMVOC (fourth row) concentrations in the IGP to meteorology (left column), emission (middle column), and combined (right column) effects. The numbers in the parenthesis show the averaged change over the colored region between April 2020 and 2019.

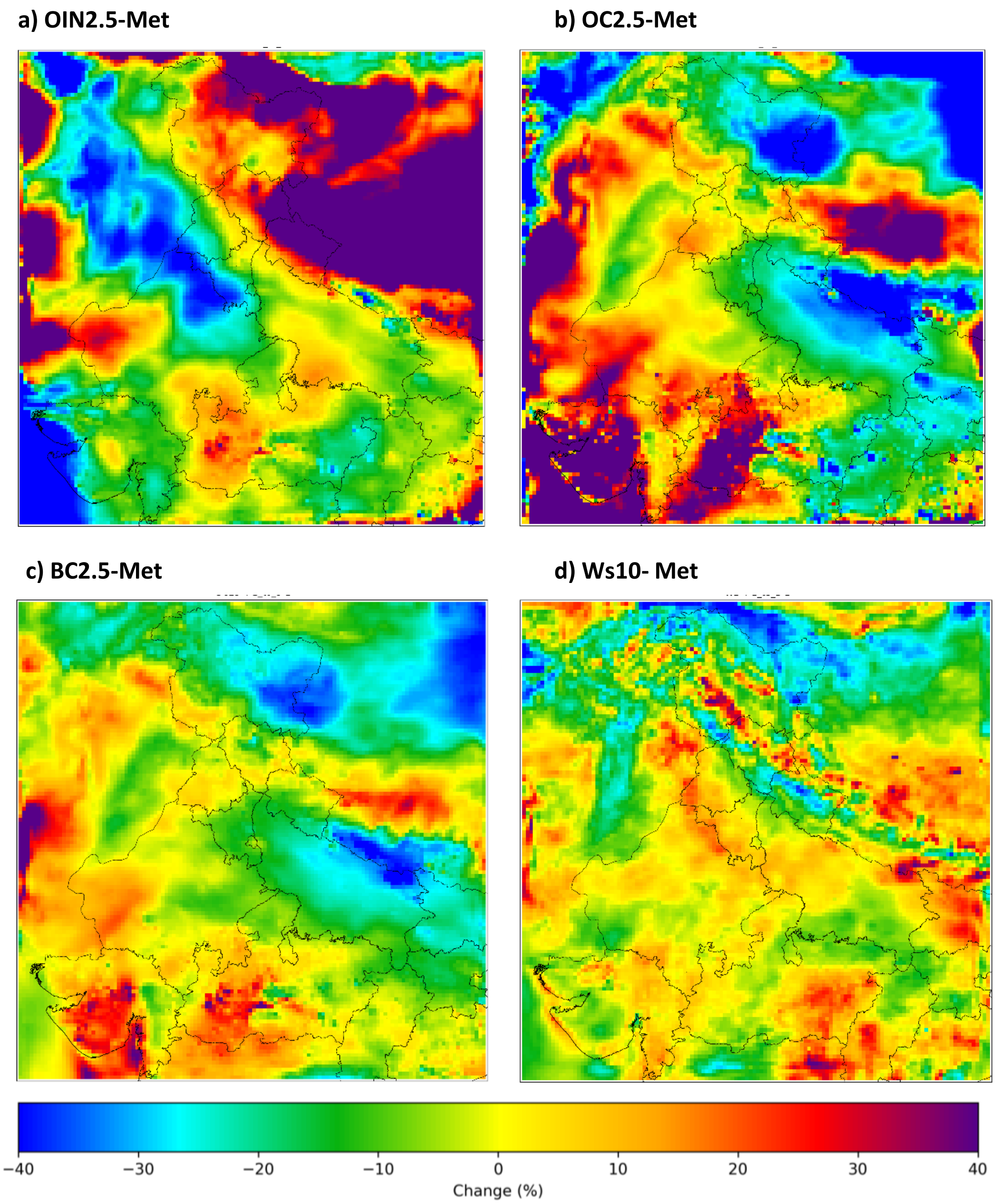

Figure S8 Responses of April averaged daytime a) other inorganics ($OIN_{2.5}$), b) $OC_{2.5}$, c) $BC_{2.5}$, and d) 10-m wind speed (Ws10) to meteorology effects.

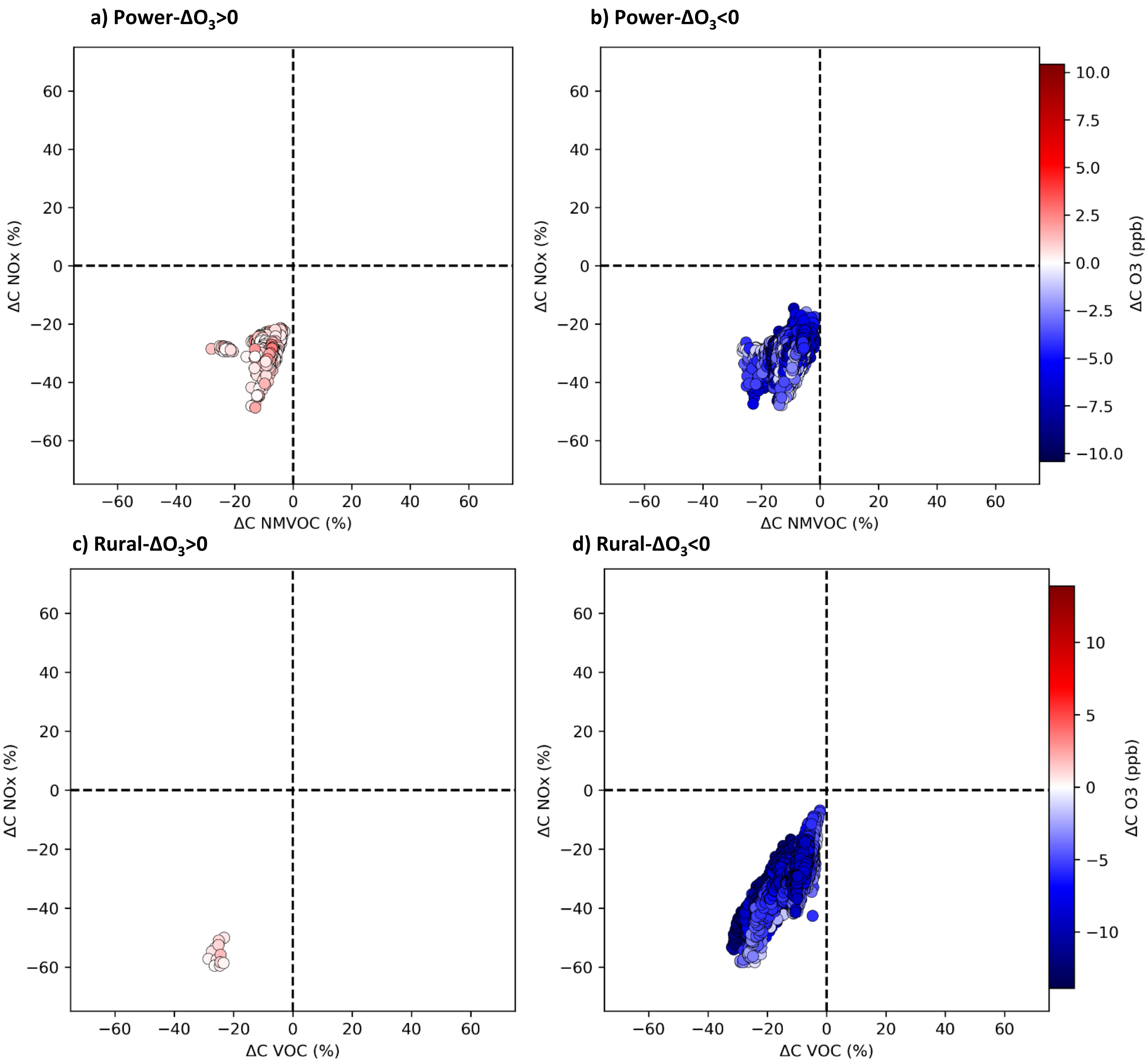

Figure S9 Plot of changes in NOx (Y-axis) and NMVOC (X-axis) concentrations due to the lockdown (2020COVID – 2020BAU) and ozone responses in all the grid cells within the Power (a, b) and Rural (c, d)regions (20 grid cells) during April (30 days) daytime (1000-1700 LT) hours (total data points are 4800). X- and Y-axis are normalized values. 5th layer in the model was selected to minimize the impacts of direct emissions.

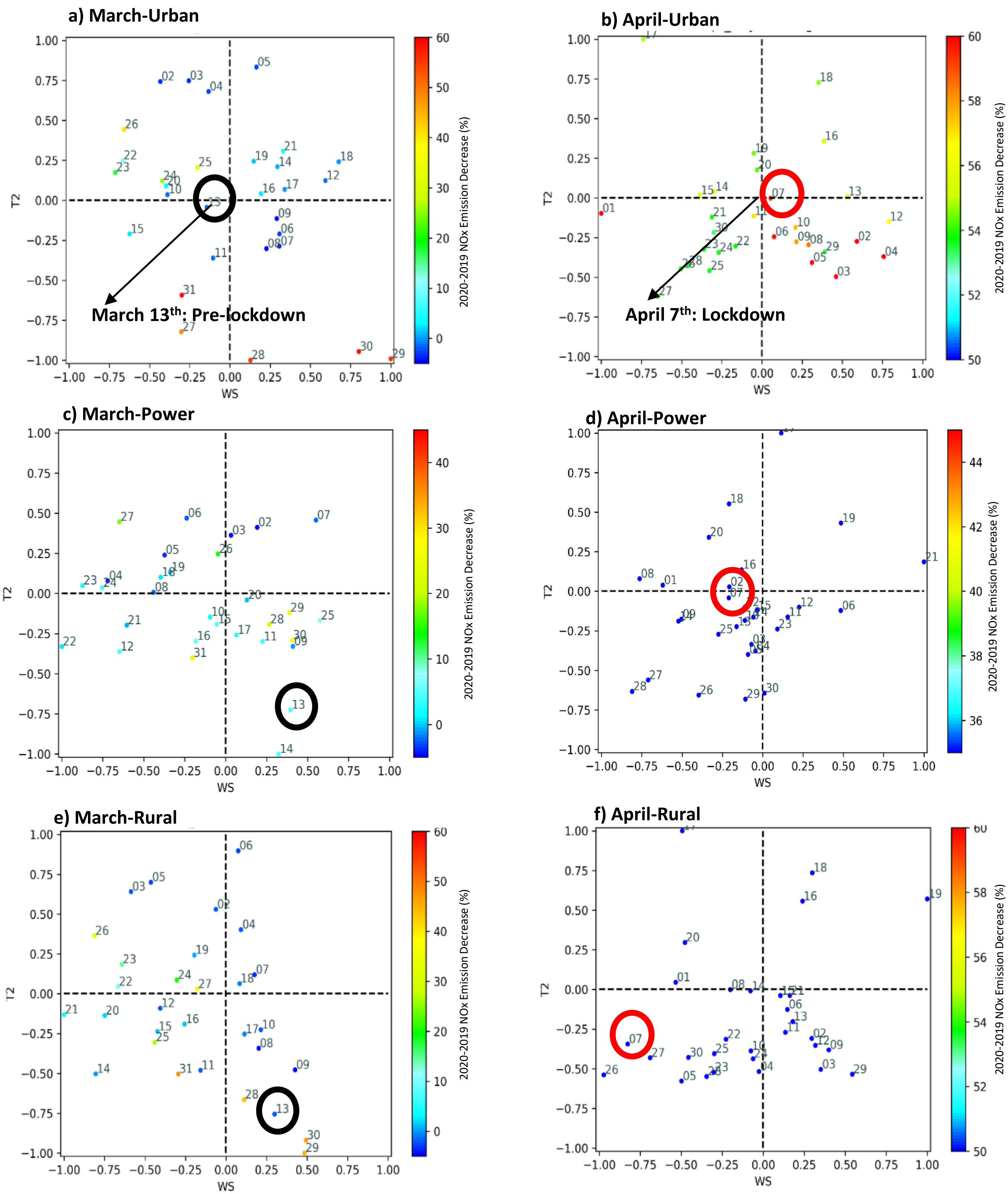

Figure S10 The changes between 2020 and 2019 in averaged daytime 2-m temperature (Y-axis) and 10-m wind speed (X-axis) in March (left column) and April (right column) in Urban (top row), Power (middle row), and Rural (bottom row). The numbers show the day of the month. The colors show the percentage of decrease in NOx emission in each day (negative value shows an increase in emission). The black (red) circle in top panel shows the day with the lowest overall changes in meteorology in March (April). X- and Y-axis are normalized changes.

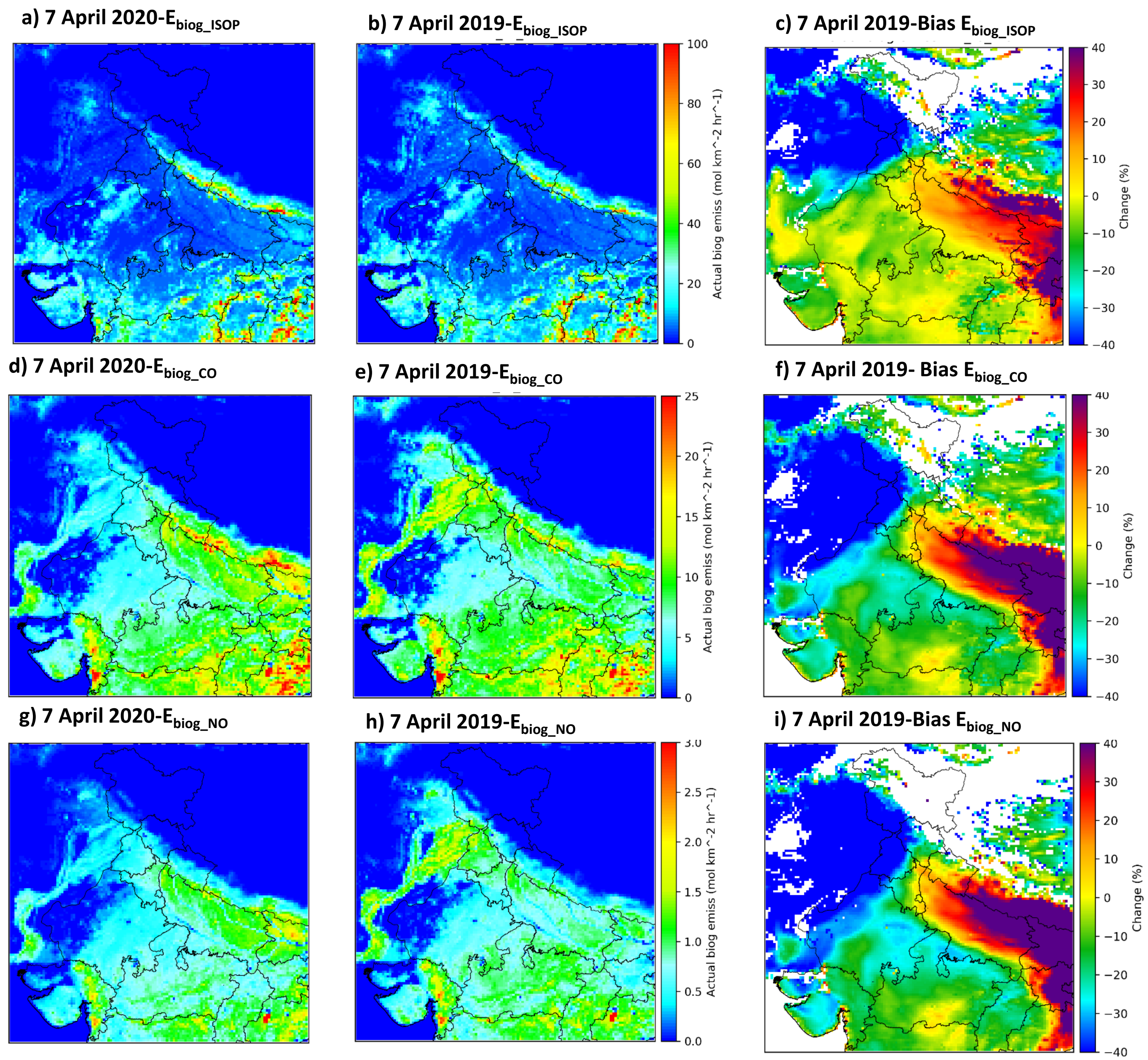

Figure S11 Biogenic emission from MEGAN in 7 April 2020 (left column) and 2019 (middle column) and their corresponding changes (right column) for isoprene (top row), CO (middle row), and NO (bottom row)

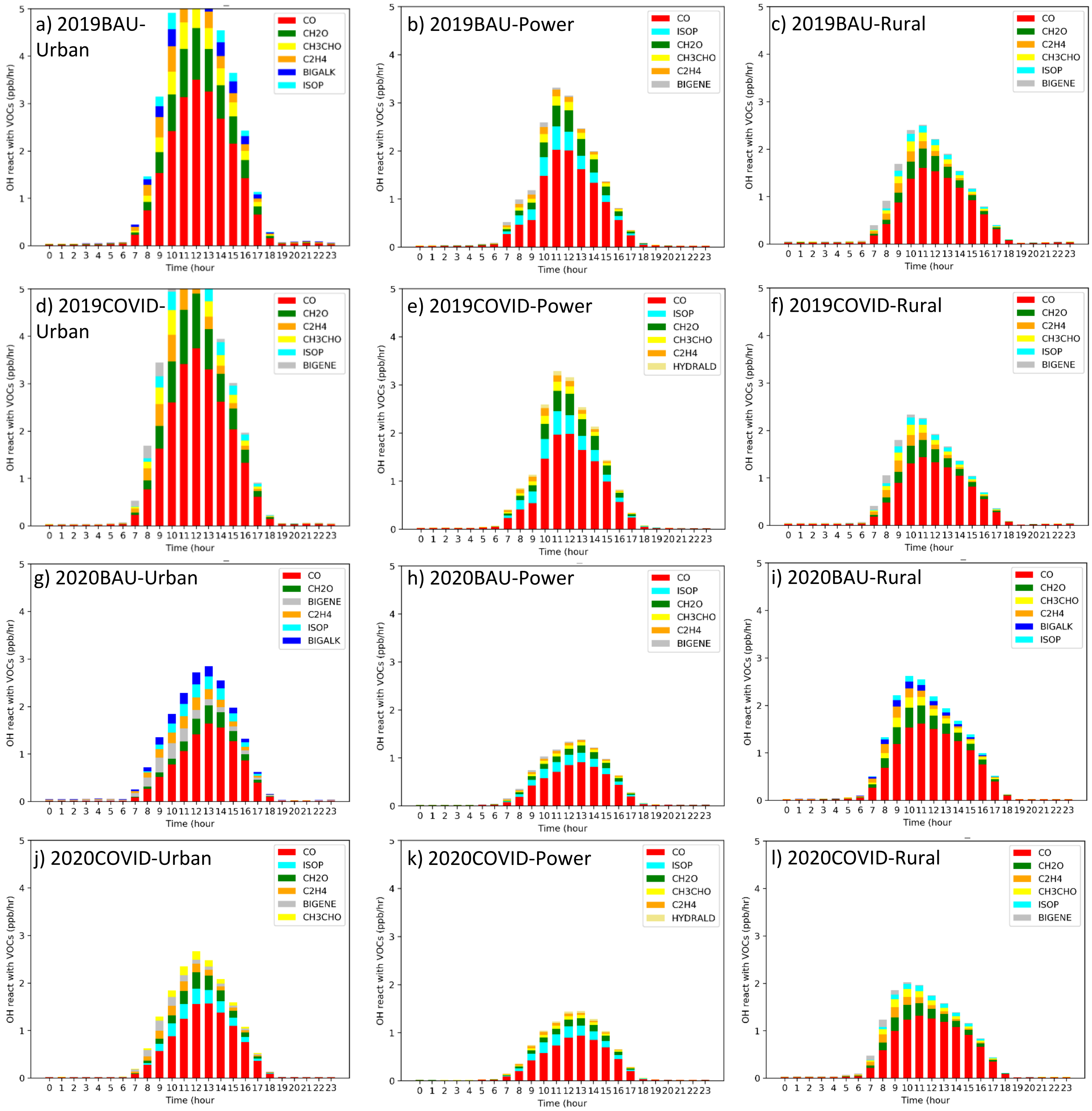

Figure S12 Diurnal cycle of OH reactivity with VOC species (averaged within the PBL) in Urban (left column), Power (middle column), and Rural (right column) for each scenario. Only the first six VOC species with higher total contribution is shown. The legend in each panel shows the ranking of the species for each scenario.

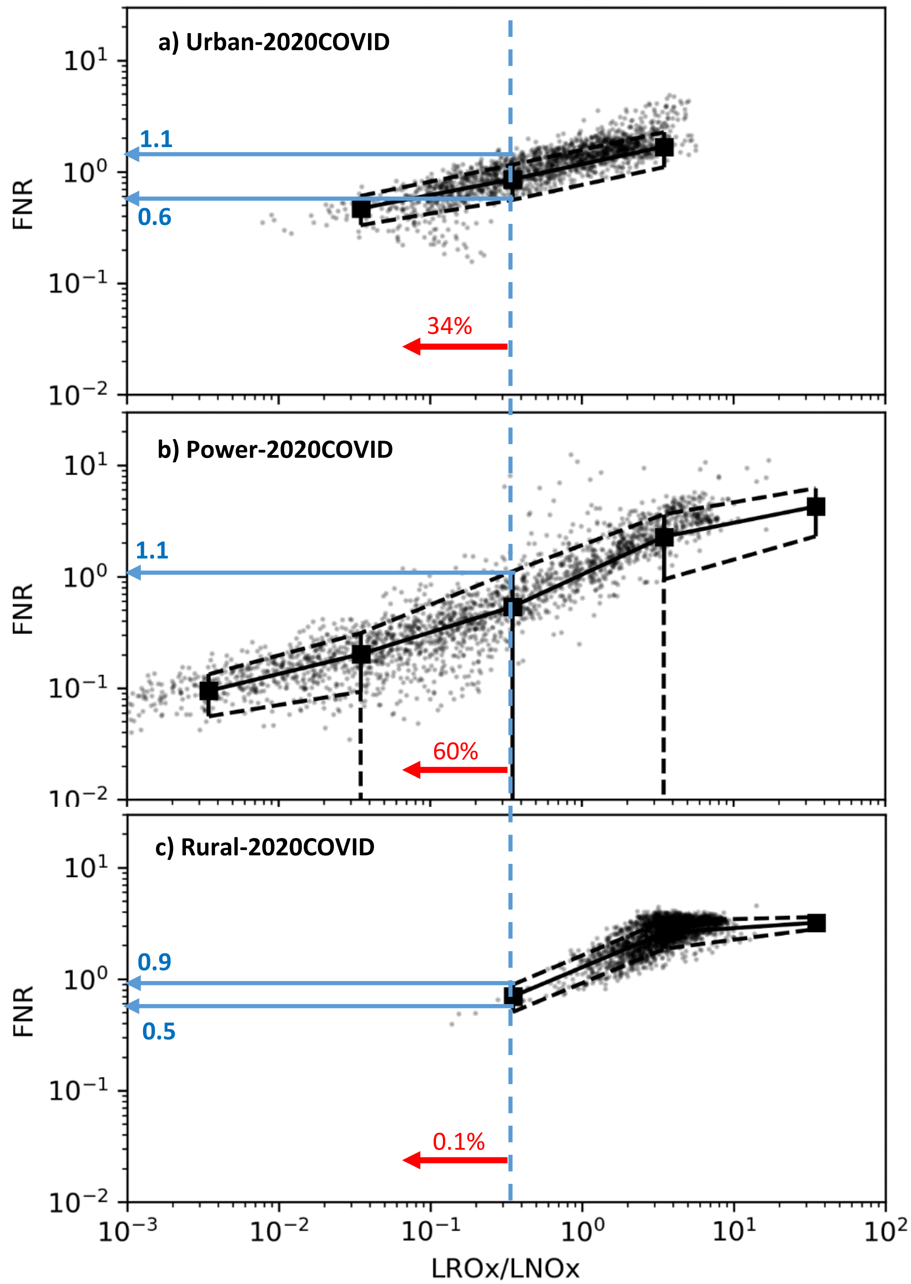

Figure S13 Plots of point-to-point FNR ratio (within the PBL) as a function of LROx/LNOx ratio during afternoon hours (1230-1430 LT) for 2020COVID scenario in a) Urban, b) Power, and c) Rural regions. Binned averages (black squares) and standard deviations (vertical black bars) were calculated. The vertical dashed blue line represents LROx/LNOx ratio of 0.35. The horizontal blue vectors show the FNR transition range in each region (numbers in blue show the values). Red values show the percentage of points in each region that fall in VOC-limited regime based on LROx/LNOx information.

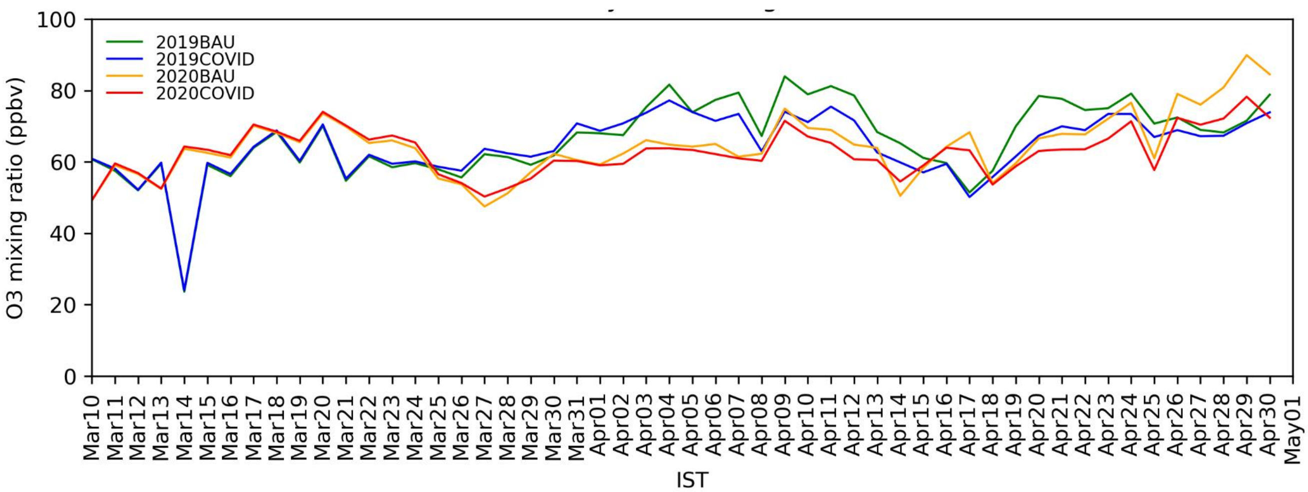

Figure S14 Daytime averaged ozone mixing ratio averaged within Urban region using all the scenarios

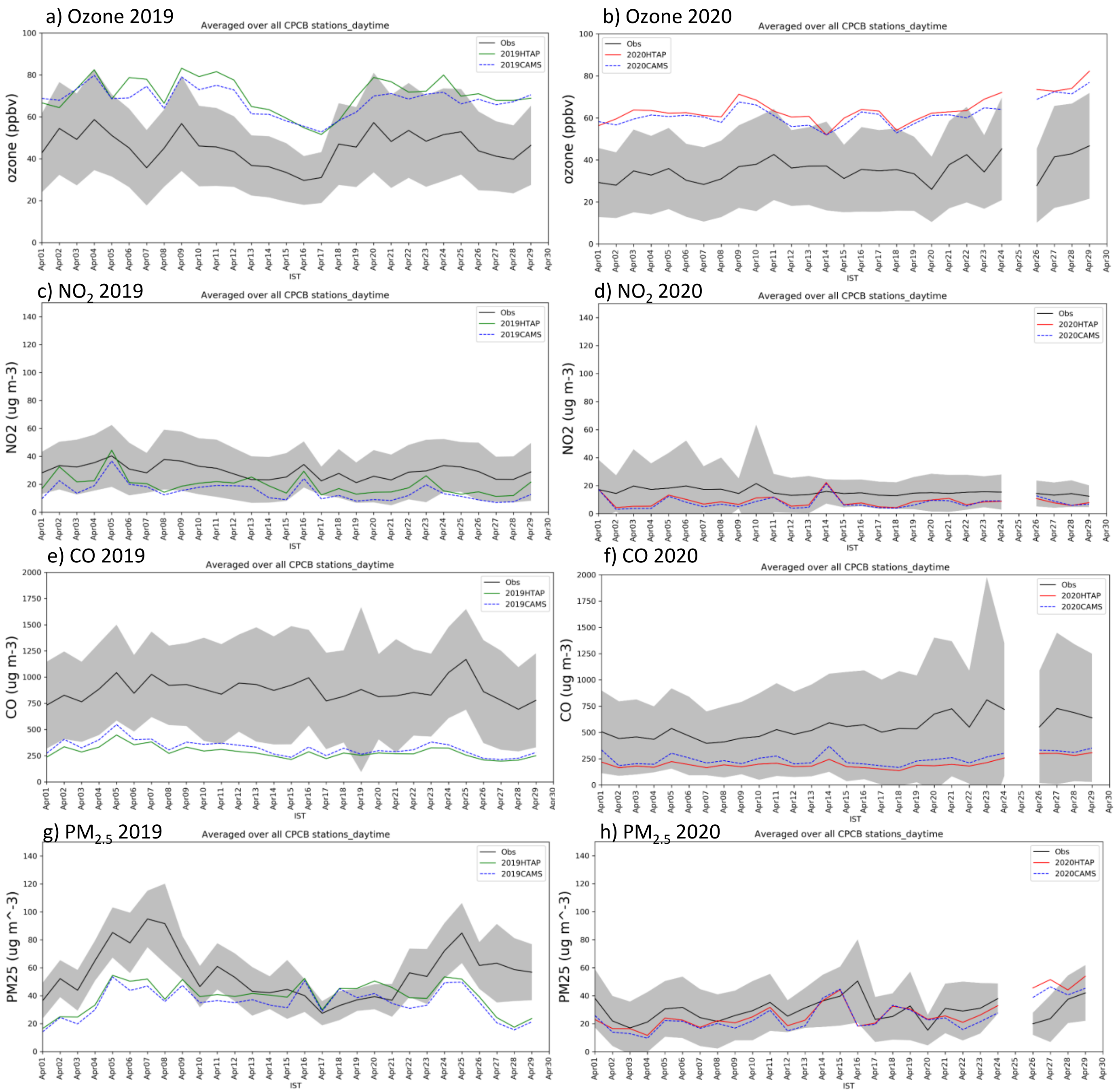

Figure S15 Simulated daytime averaged and measured data in CPCB stations in Delhi for ozone, NO_2, CO, and $PM_{2.5}$ concentrations using HTAP and CAMS emission inventories in April 2019 (left column) and 2020 (right column). Shaded area shows 1STD of the measured values.

Table S1 The mapping between HTAP and CAMS VOC species to MOZART mechanism in WRF-Chem

MOZART	HTAP	CAMS
C2H2	ethyne	voc9
C2H4	ethene	voc7
C2H6	ethane	voc2
C3H6	propene	voc8
C3H8	propane	voc3
BIGALK	butanes + pentanes + hexanes&higher-alkanes + esters + ethers	voc4+voc5+voc6+voc18+voc19
BIGENE	other-alkenes	voc12
BENZENE	benzene	voc13
TOLUENE	toluene	voc14
XYLENES	xylene + trimethylbenzenes + other-aromatics	voc15+voc16+voc17
CH2O	methanal	voc21
CH3CHO	other-alkanals (aldehydes)	voc22
CH3OH	0.15 * alcohols	0.15*voc1
C2H5OH	0.85 * alcohols	0.85*voc1
CH3COCH3	0.2 * ketones	0.2*voc23
MEK	0.8 * ketones	0.8*voc23
HCOOH	0.5 * acids	0.5*voc24
CH3COOH	0.5 * acids	0.5*voc24
ISOP		voc10
C10H16		voc11

Table S2 Total emissions in HTAP inventory using BAU and COVID scenarios in March

	India		Urban		Power		Rural	
Species (unit)	BAU	COVID	BAU	COVID	BAU	COVID	BAU	COVID
NMVOC (Gmol)	14.23	13.8	0.45	0.4	0.03	0.03	0.04	0.04
NOx (Gmol)	9.52	8.69	0.49	0.43	0.42	0.4	0.01	0.013
CO (Gmol)	119.0	115.53	2.47	2.18	0.98	0.94	0.26	0.26
SO2 (Gmol)	7.22	6.75	0.18	0.17	0.46	0.44	0.00	0.00
BC (Tg)	45.54	45.66	0.69	0.62	0.09	0.09	0.08	0.08
OC (Tg)	106.75	111.14	0.76	0.73	0.18	0.19	0.23	0.24

Table S3 Total emissions in HTAP inventory using BAU and COVID scenarios in April

	India		Urban		Power		Rural	
Species (unit)	BAU	COVID	BAU	COVID	BAU	COVID	BAU	COVID
NMVOC (Gmol)	13.28	11.14	0.42	0.19	0.03	0.02	0.04	0.03
NOx (Gmol)	8.82	5.21	0.46	0.2	0.38	0.29	0.01	0.007
CO (Gmol)	110.9	93.59	2.28	1.05	0.9	0.69	0.25	0.21
SO2 (Gmol)	6.6	4.49	0.17	0.11	0.42	0.32	0.00	0.00
BC (Tg)	42.15	41.44	0.63	0.34	0.08	0.09	0.08	0.09
OC (Tg)	99.3	114.38	0.7	0.55	0.17	0.20	0.22	0.26

Table S4 Daytime (1000-1700 LT) statistics. Mean (± standard deviation), Normalized Mean Bias (NMB), Root Mean Square Error (RMSE), and Pearson Correlation Coefficient averaged for all CPCB stations in Delhi in 2019 (scenario: 2019BAU) and 2020 (scenario: 2020COVID) using HTAP and CAMS anthropogenic emission inventories.

			HTAP				**CAMS**			
Variable	Year	OBS Mean (±1std)	*MODEL Mean (±1std)*	*NMB (%)*	*RMSE*	*R (%)*	MODEL Mean (±1std)	NMB (%)	RMSE	R (%)
O_3 (ppb)	2019	50(±11)	*71(±13)*	*+43*	*25*	*+37*	69(±11)	+38	22	+38
	2020	36(±6)	*64(±9)*	*+78*	*30*	*+37*	62(±8)	+70	27	+36
$PM_{2.5}$ (µg/m3)	2019	56(±22)	*39(±12)*	*-31*	*27*	*+36*	34(±12)	-39	30	+44
	2020	30(±13)	*28(±12)*	*-7*	*14*	*+42*	25(±11)	-17	13	+47
NO_2 (µg/m3)	2019	28(±7)	*18(±13)*	*-35*	*15*	*+38*	13(±11)	-55	18	+43
	2020	14(±2)	*7(±7)*	*-47*	*9*	*+33*	6(±7)	-56	10	+30
CO (µg/m3)	2019	829(±135)	*277(±86)*	*-67*	*566*	*+42*	305(±109)	-63	541	+40
	2020	566(±132)	201(±57)	-64	382	+53	237(±83)	-58	351	+43

Table S5 24-hour averages statistics. Mean (± standard deviation), Normalized Mean Bias (NMB), Root Mean Square Error (RMSE), and Pearson Correlation Coefficient averaged for all CPCB stations in Delhi in 2019 (scenario: 2019BAU) and 2020 (scenario: 2020COVID) using HTAP and CAMS anthropogenic emission inventories. 17285 and 22880 hourly points prior to applying filters were used in 2019 and 2020, respectively.

			HTAP				**CAMS**			
Variable	Year	OBS Mean (±1std)	*MODEL Mean (±1std)*	*NMB (%)*	*RMSE*	*R (%)*	MODEL Mean (±1std)	NMB (%)	RMSE	R (%)
O_3 (ppb)	2019	27(±20)	*31(±32)*	*+18*	*19*	*+87*	37(±27)	+38	17	+85
	2020	24(±12)	*35(±25)*	*+47*	*20*	*+84*	38(±20)	+59	19	+82
$PM_{2.5}$ (µg/m3)	2019	82(±40)	*56(±20)*	*-31*	*42*	*+53*	59(±26)	-28	40	+57
	2020	45(±23)	*38(±15)*	*-17*	*21*	*+51*	41(±19)	-9	19	+60
NO_2 (µg/m3)	2019	46(±20)	*70(±45)*	*+51*	*42*	*+68*	56(±40)	+22	34	+60
	2020	20(±7)	*42(±32)*	*+116*	*36*	*+61*	34(±27)	+72	27	+54
CO (µg/m3)	2019	1095(±369)	*563(±270)*	*-49*	*622*	*+53*	685(±356)	-37	539	+53
	2020	670(±179)	*339(±136)*	*-49*	*363*	*+58*	516(±261)	-23	266	+56

Table S6 Reactions used to calculate the LROx in IRR analysis

MOZART Reactions	**IRR reactions (LROx)**
ALKO2 + HO2 -> ALKOOH	ALKO2_HO2_IRR
BENZO2 + HO2 -> BENZOOH	BENZO2_HO2_IRR
BZOO + HO2 -> BZOOH	BZOO_HO2_IRR
C2H5O2 + HO2 -> C2H5OOH + O2	C2H5O2_HO2_IRR
C3H7O2 + HO2 -> C3H7OOH + O2	C3H7O2_HO2_IRR
C6H5O2 + HO2 -> C6H5OOH	C6H5O2_HO2_IRR
CH3O2 + HO2 -> CH3OOH + O2	CH3O2_HO2_IRR
HO2 + HO2 -> H2O2 + O2	HO2_HO2_H2O_IRR
HO2 + aer -> 0.5*H2O2	HO2_IRR
HOCH2OO + HO2 -> HCOOH	HOCH2OO_HO2_IRR
ISOPAO2 + HO2 -> ISOPOOH	ISOPO2_HO2_IRR
MACRO2 + HO2 -> MACROOH	MACRO2_HO2_IRR
MBONO3O2 + HO2 ->	MBONO3O2_HO2_IRR
MBOO2 + HO2 -> MBOOOH	MBOO2_HO2_IRR
MEKO2 + HO2 -> MEKOOH	MEKO2_HO2_IRR
NTERPO2 + HO2 -> NTERPOOH	NTERPO2_HO2_IRR
OH + HO2 -> H2O + O2	OH_HO2_IRR
PHENO2 + HO2 -> PHENOOH	PHENO2_HO2_IRR
PO2 + HO2 -> POOH + O2	PO2_HO2_IRR
RO2 + HO2 -> ROOH	RO2_HO2_IRR
TERP2O2 + HO2 -> TERP2OOH	TERP2O2_HO2_IRR
TERPO2 + HO2 -> TERPOOH	TERPO2_HO2_IRR
TOLO2 + HO2 -> TOLOOH	TOLO2_HO2_IRR
XO2 + HO2 -> XOOH	XO2_HO2_IRR
XYLENO2 + HO2 -> XYLENOOH	XYLENO2_HO2_IRR
XYLOLO2 + HO2 -> XYLOLOOH	XYLOLO2_HO2_IRR

Table S7 Reactions used to calculate the LNOx in IRR analysis

MOZART Reactions	IRR reactions
CH3CO3 + NO2 + M -> PAN + M	CH3CO3_NO2_IRR
DICARBO2 + NO2 + M -> NDEP + M	DICARBO2_NO2_IRR
MACRO2 + NO -> .8 ONITR + nume	MACRO2_NO_a_IRR
MALO2 + NO2 + M -> NDEP + M	MALO2_NO2_IRR
MDIALO2 + NO2 + M -> NDEP + M	MDIALO2_NO2_IRR
NO2 + OH + M -> HNO3 + M	OH_NO2_IRR
PHENO + NO2 -> NDEP	PHENO_NO2_IRR

Table S8 Total OH reactivity with VOCs and NO2 and corresponding ration in Urban, Power, and Rural for April 7th (lockdown sample day)

Scenario	OH+VOC	OH+NO2	(OH+VOC)/(OH+NO2)
Urban			
2019BAU	58.67	13.75	4.27
2019COVID	54.03	8.15	6.63
2020BAU	27.3	8.2	3.3
2020COVID	23.28	4.59	5.07
Power			
2019BAU	24.23	7.65	3.17
2019COVID	23.91	6.22	3.84
2020BAU	12.21	6.63	1.84
2020COVID	12.61	5.8	2.17
Rural			
2019BAU	20.78	2.68	7.75
2019COVID	19.62	1.78	11.02
2020BAU	24.21	2.27	10.67
2020COVID	19.74	1.25	15.79

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