Supplement of Atmos. Chem. Phys., 17, 14393–14413, 2017
https://doi.org/10.5194/acp-17-14393-2017-supplement

Atmospheric Chemistry and Physics
Open Access
EGU

Supplement of

WRF-Chem simulated surface ozone over south Asia during the pre-monsoon: effects of emission inventories and chemical mechanisms

Amit Sharma et al.

Correspondence to: Amit Sharma (amit.iit87@gmail.com) and Narendra Ojha (narendra.ojha@mpic.de)

Supplementary material

WRF-Chem simulated surface ozone over South Asia during the pre-monsoon: Effects of emission inventories and chemical mechanisms

Amit Sharma[1, 2, *], Narendra Ojha[2, *], Andrea Pozzer[2], Kathleen A. Mar[3], Gufran Beig[4], Jos Lelieveld[2, 5], and Sachin S. Gunthe[1]

[1]Department of Civil Engineering, Indian Institute of Technology Madras, Chennai, India
[2]Atmospheric Chemistry Department, Max Planck Institute for Chemistry, Mainz, Germany
[3]Institute for Advanced Sustainability Studies, Potsdam, Germany
[4]Indian Institute for Tropical Meteorology, Pune, India
[5]Energy, Environment and Water Research Center, The Cyprus Institute, Nicosia, Cyprus

[*]Correspondence to Amit Sharma (amit.iit87@gmail.com) and Narendra Ojha (narendra.ojha@mpic.de)

Table S1. Comparison of modeled monthly average (for April) precursor mixing ratios (in ppbv) with observations at several stations.

Specie	Site	Reference	Observations ±1 σ std	HTAP-RADM2	INTEX-RADM2	S4RS-RADM2	HTAP-MOZ
NOx	Delhi	SAFAR data	59.8±27.5	208.7	64.4	187.2	188.9
	Kanpur	Gaur et al. (2014)	5.0	10.2	6.5	30.5	9.1
	Udaipur	Yadav et al. (2014)	8.7±4.2	2.1	1.6	1.5	2.0
NOy	Nainital	Sarangi et al. (2014)	1.8±1.6	3.2	2.7	2.9	2.6
NMVOC (*ethane*)	Nainital	Sarangi et al. (2016)	2.3	1.2	1.2	1.1	1.0
NMVOC (*ethene*)	Nainital	Sarangi et al. (2016)	0.9	1.2	0.9	0.8	0.9

Table S2. Diurnal mean biases (model-observations) for surface ozone mixing ratio in ppbv for all runs at different sites.

Site	HTAP-RADM2	INTEX-RADM2	S4RS-RADM2	HTAP-MOZ
Mohali	-3.4	-5.5	-9.4	1.0
Nainital	0.6	-2.0	-1.2	8.3
Pantnagar	17.8	15.1	16.1	24.7
Delhi	-6.5	-5.4	-12.3	-16.0
Dibrugarh	21.6	20.6	16.8	39.1
Kanpur	18.2	11.4	10.0	17.8
Udaipur	11.8	10.3	9.7	11.4
Jabalpur	-10.2	-15.1	-12.4	-2.1
Ahmedabad	8.7	8.1	7.8	3.7
Bhubaneshwar	6.4	4.8	4.8	13.1
Pune	5.1	2.2	4.7	6.9
Anantpur	-5.3	-12.9	-11.2	4.8
Gadanki	7.1	3.2	3.8	11.6
Kannur	15.7	13.4	12.7	13.6
Thumba/Trivendrum	11.7	9.9	6.1	12.0

Table S3. Noontime (1130-1630 IST) average biases for surface ozone mixing ratio in ppbv for all runs at different sites.

Site	HTAP-RADM2	INTEX-RADM2	S4RS-RADM2	HTAP-MOZ
Mohali	-17.6	-20.8	-24.8	-13.5
Nainital	8.1	5.8	6.2	17.0
Pantnagar	10.5	7.4	8.5	20.4
Delhi	-12.3	-21.5	-26.0	-11.3
Dibrugarh	28.8	31.5	24.6	40.7
Kanpur	23.5	12.5	15.7	28.7
Udaipur	9.4	7.5	6.8	10.7
Jabalpur	0.9	-8.0	-2.5	8.8
Ahmedabad	10.7	9.4	6.9	10.7
Bhubaneshwar	10.2	12.2	7.3	19.9
Pune	10.5	4.4	10.5	15.2
Anantpur	0.2	-10.0	-8.7	13.5
Gadanki	14.6	7.9	8.7	25.2
Kannur	22.5	14.9	15.0	27.4
Thumba/Trivendrum	24.0	19.9	11.1	35.8

Table S4. Diurnal mean biases for surface ozone mixing ratio in ppbv over different regions in all model runs.

Region	HTAP-RADM2	INTEX-RADM2	S4RS-RAMD2	HTAP-MOZ
North	5.4	2.7	0.6	9.4
East	14.0	12.7	10.8	21.8
West	8.6	6.9	7.4	5.4
Central	-10.2	-15.1	-12.4	-2.1
South	7.3	3.4	2.9	10
Overall	6.6	4.1	3.1	9.6

Table S5. A comparison of noontime (1130-1630 IST) average mean biases for surface ozone mixing ratio in ppbv over different regions for the four simulations.

Region	HTAP-RADM2	INTEX-RADM2	S4RS-RADM2	HTAP-MOZ
North	2.4	-3.3	-4.1	8.3
East	19.5	21.9	15.9	30.3
West	10.2	7.1	8.1	12.2
Central	0.9	-8.0	-2.5	8.8
South	15.3	8.2	6.5	25.5
Overall	9.6	4.9	3.9	16.6

Table S6. Quantitative assessment of similarity between HTAP-RAMD2, INTEX-RADM2 and SEAC4RS-RADM2 scenarios for 24 h average and noontime (1130-1630 IST) average for simulated surface ozone mixing ratios.

24 h average	**HTAP-RADM2 (a) vs INTEX-RADM2 (b)**	**HTAP-RADM2 (a) vs S4RS-RADM2 (b)**	**INTEX-RADM2 (a) vs S4RS-RADM2 (b)**
r^2	0.98	0.98	0.99
variance of the residual (b-a)	4.61	5.32	2.05
Noontime average			
r^2	0.96	0.96	0.98
variance of the residual (b-a)	18.26	21.24	11.70

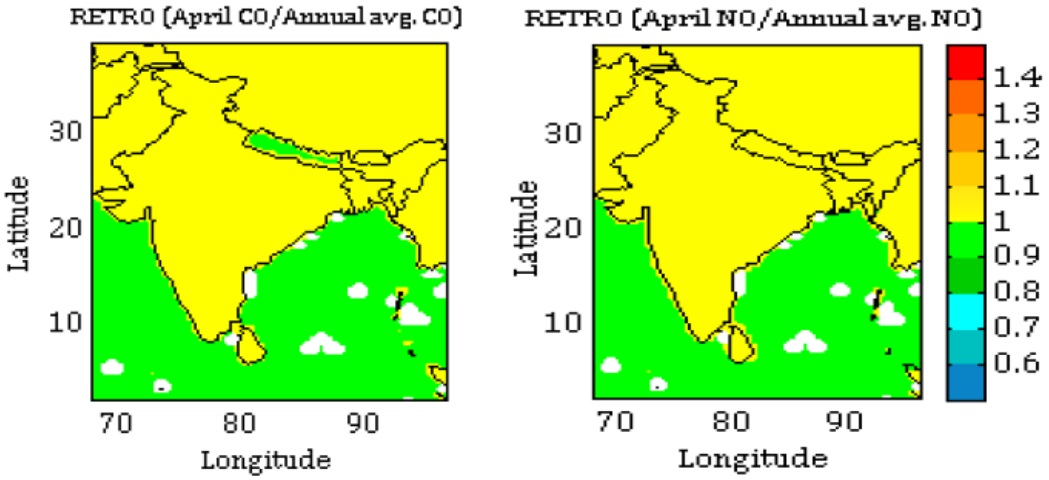

Figure S1. Spatial distribution of ratio of April emissions to annual average emissions for CO (left) and NO (right) derived from the RETRO inventory (http://accent.aero.jussieu.fr/RETRO_metadata.php).

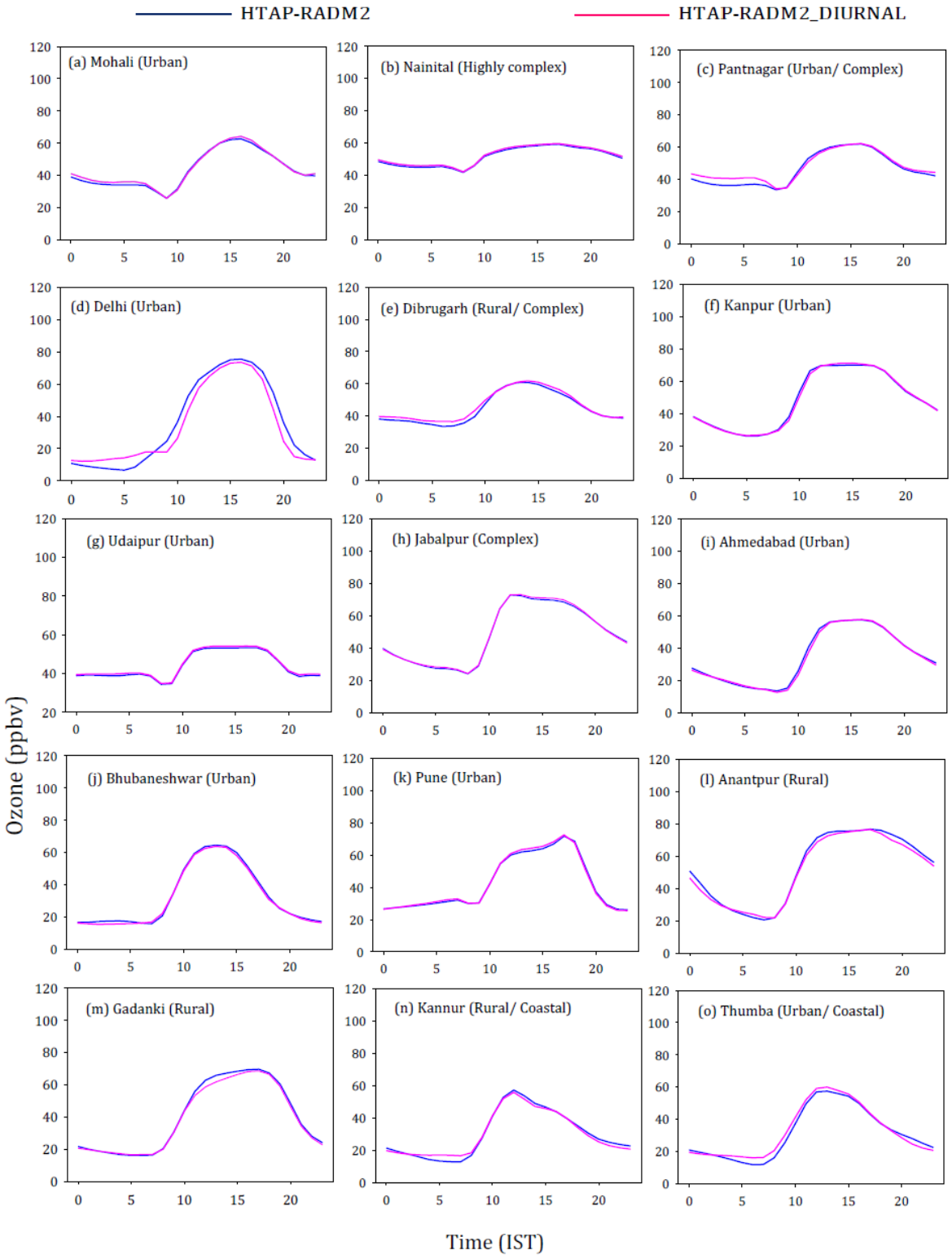

Figure S2. Comparison of 15 day average (01st April, 2013 – 15th April, 2013) diurnal variation of surface ozone simulated for anthropogenic emissions with and without the incorporation of diurnal profile of emissions at various observation sites. Both model simulations are with the HTAP inventory and RADM2 chemistry option.

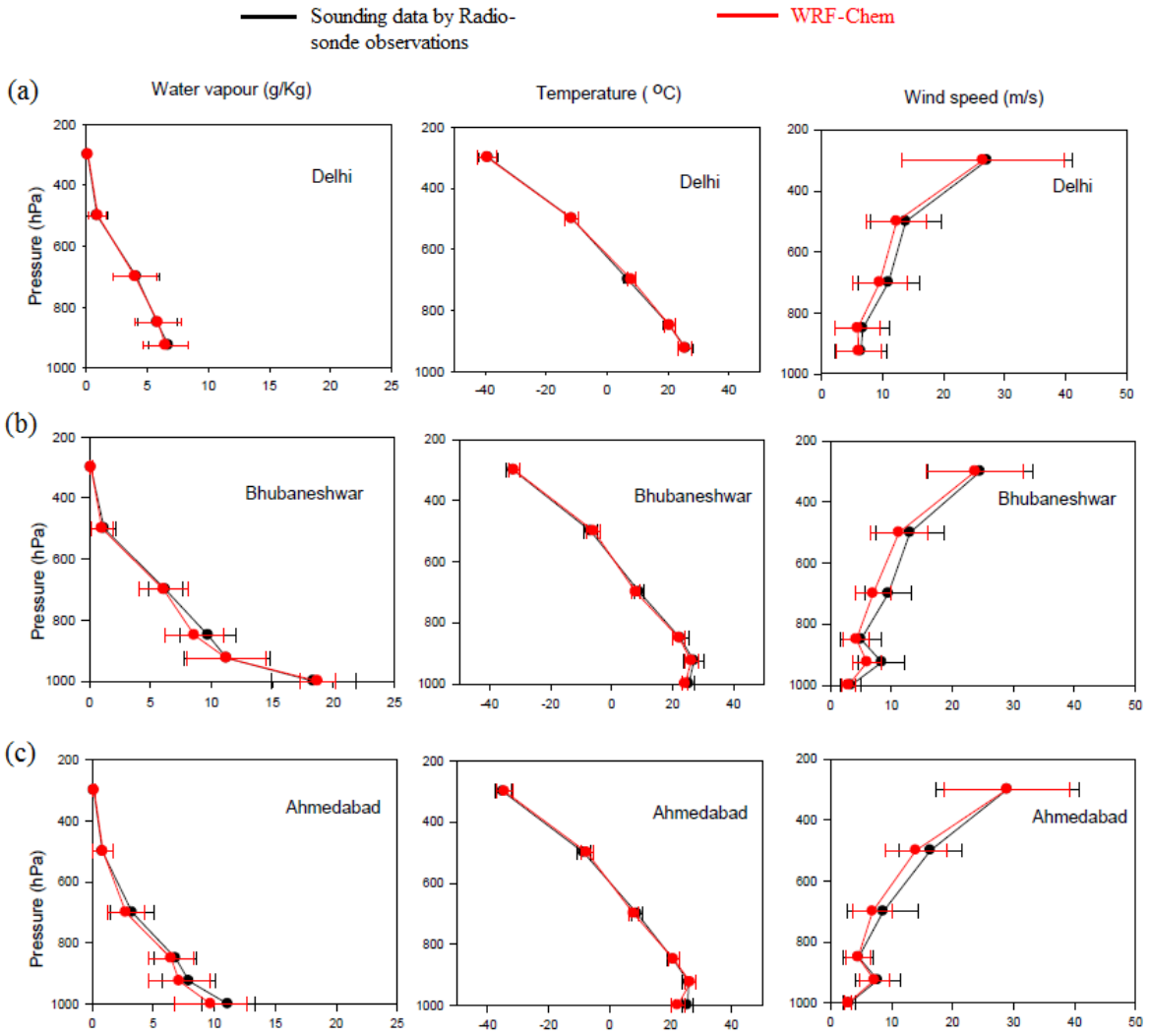

Figure S3. Vertical profiles of monthly average (April 2013) water vapour mixing ratio (g/Kg), temperature (^{o}C) and wind speed (m/s) from WRF-Chem (in red) and sounding data (in black) at (a) Delhi (in north India); (b) Bhubaneshwar (in east India); and, (c) Ahmedabad (in west India). Horizontal bars represent temporal standard deviation of monthly averages.

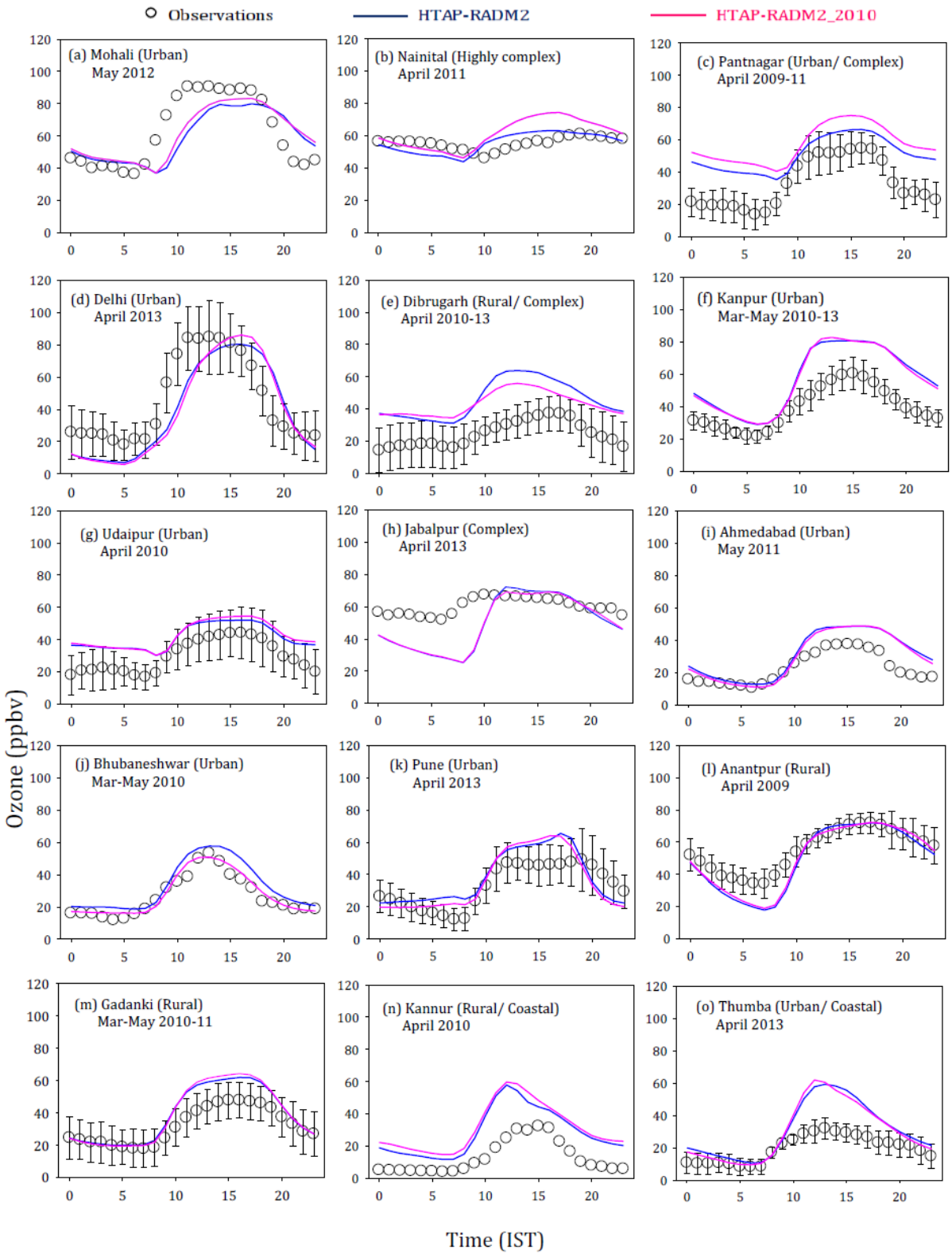

Figure S4. Comparison of monthly average diurnal variation of surface ozone simulated for the years 2010 and 2013 at various observation sites. The observational data is available for the period indicated in the figure. Error bars represent the temporal standard deviation of the monthly averages. All model simulations are with the HTAP inventory and RADM2 chemistry option.

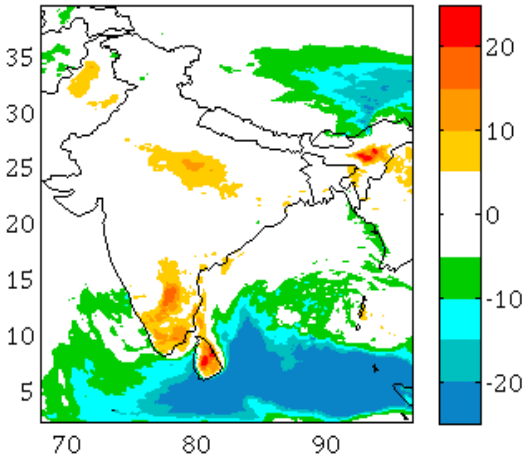

Figure S5. Percentage difference in monthly average surface ozone mixing ratio (ppbv) during April between S4RS-RADM2_kf run (using Kain-Fritsch cumulus parameterization scheme) and S4RS-RADM2 i.e. base run (using Grell 3D scheme). The percentage difference is calculated relative to base run.

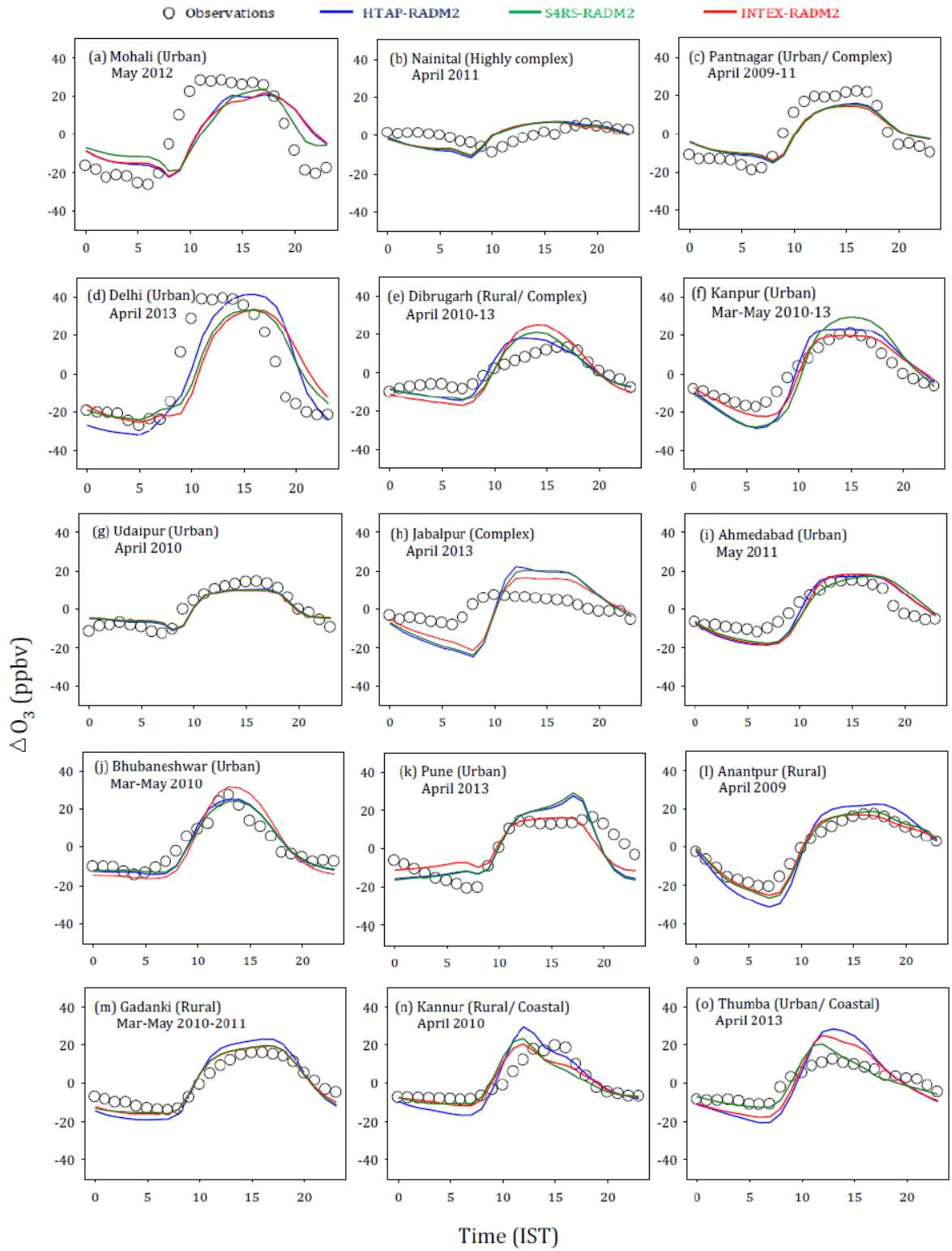

Figure S6. Comparison of monthly average diurnal variation of delta surface ozone (ΔO3), which is the difference between diurnal mean and hourly values, using different emission inventories at various observation sites. Units are in ppbv. All model simulations are with RADM2 chemistry.

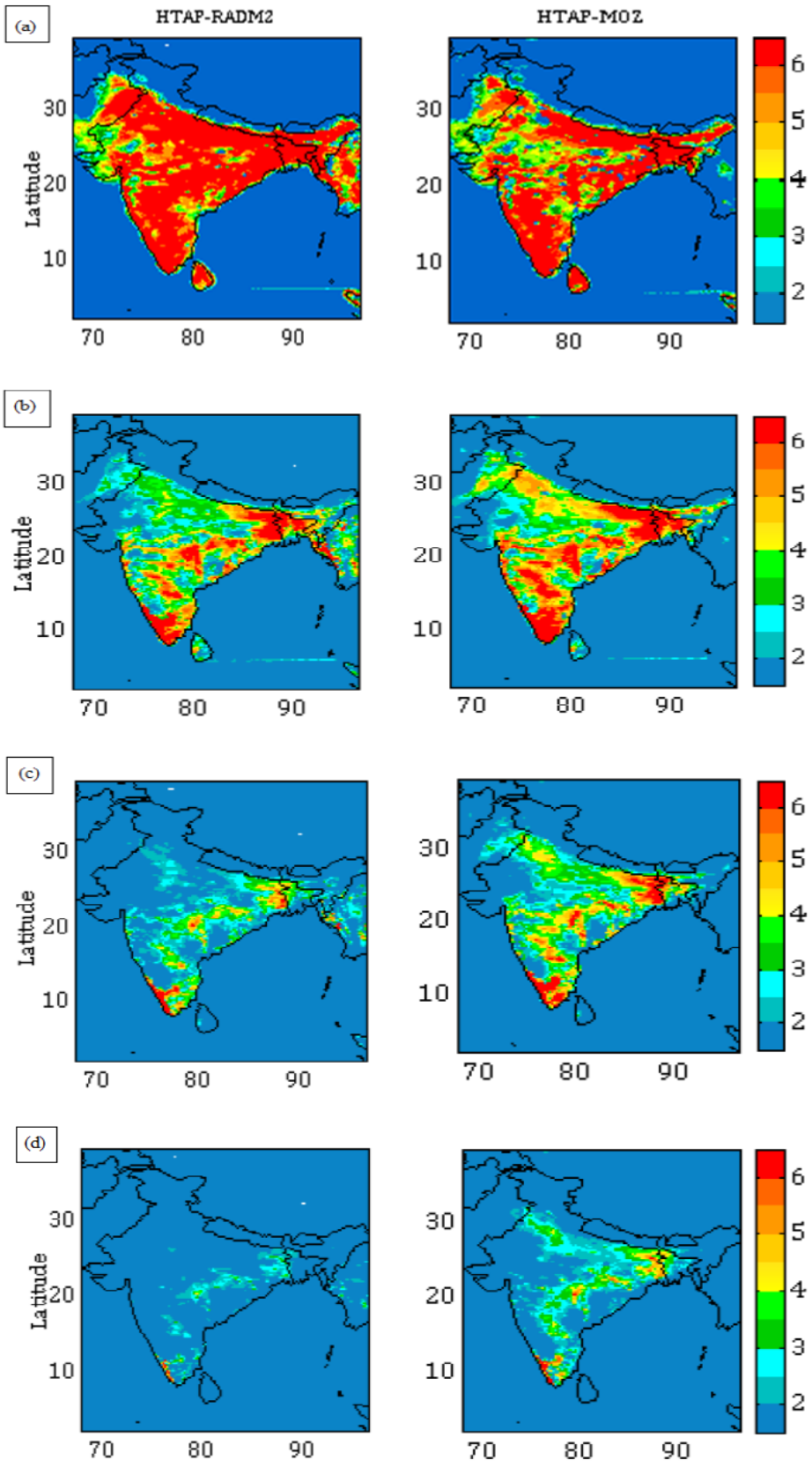

Figure S7. Spatial distribution of net daytime ozone chemical tendency (in ppbv h^{-1}) at model (a)level 1 - surface; (b) level 4; (c) level 5; and (d) level 6 during 0630-1230 IST. The pressure distribution at these model levels is shown in figure S9. Note the colour scale difference with respect to Fig. 9 in the manuscript.

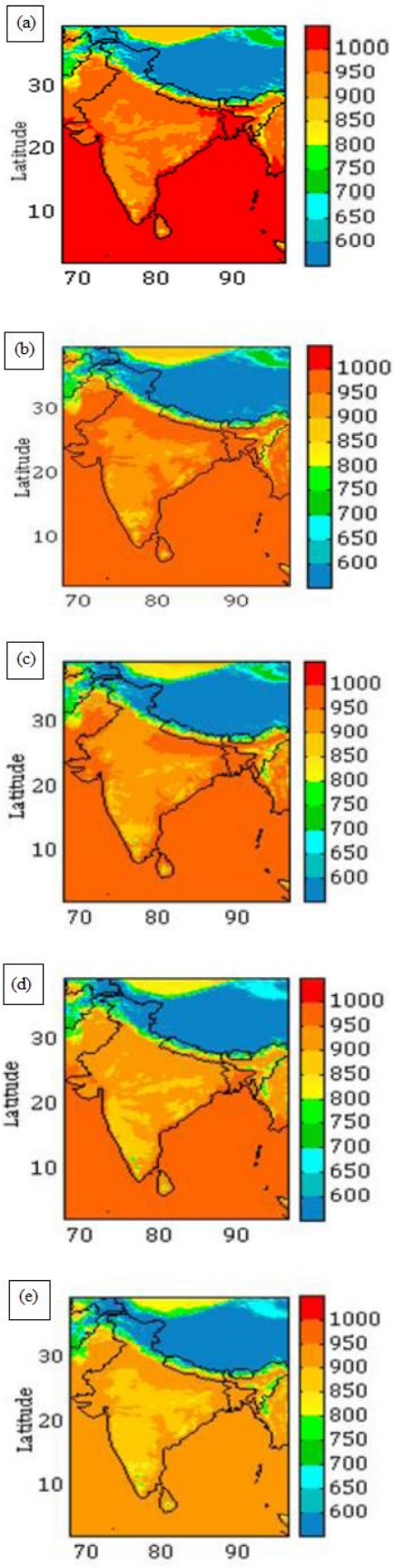

Figure S8. Spatial distribution of atmospheric pressure (in hPa) at model (a) level 1 - surface; (b) level 3; (c) level 4; (d) level 5 and (e) level 6.

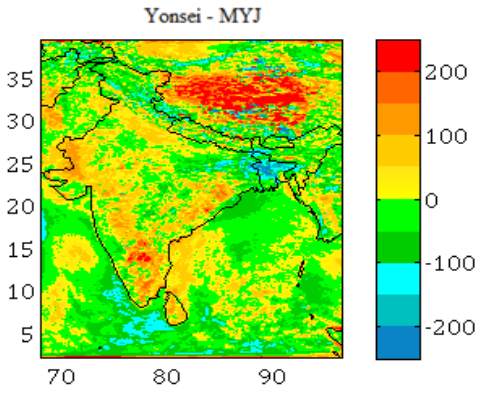

Figure S9. Difference in monthly average (in April) PBL height in meters between simulations with Yonsei and MYJ parameterization (i.e. base run) with HTAP-RADM2 setup.

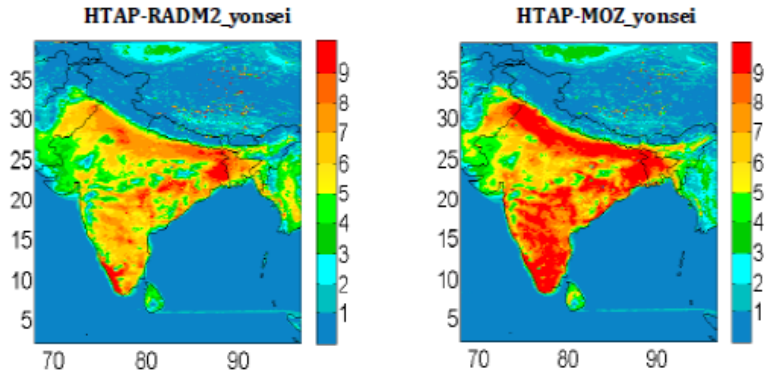

Figure S10. Average net daytime surface ozone chemical +vertical mixing tendency (in ppbv h^{-1}) for April during 0630-1230 IST for HTAP-RADM2 and HTAP-MOZ setup but with the Yonsei PBL scheme.

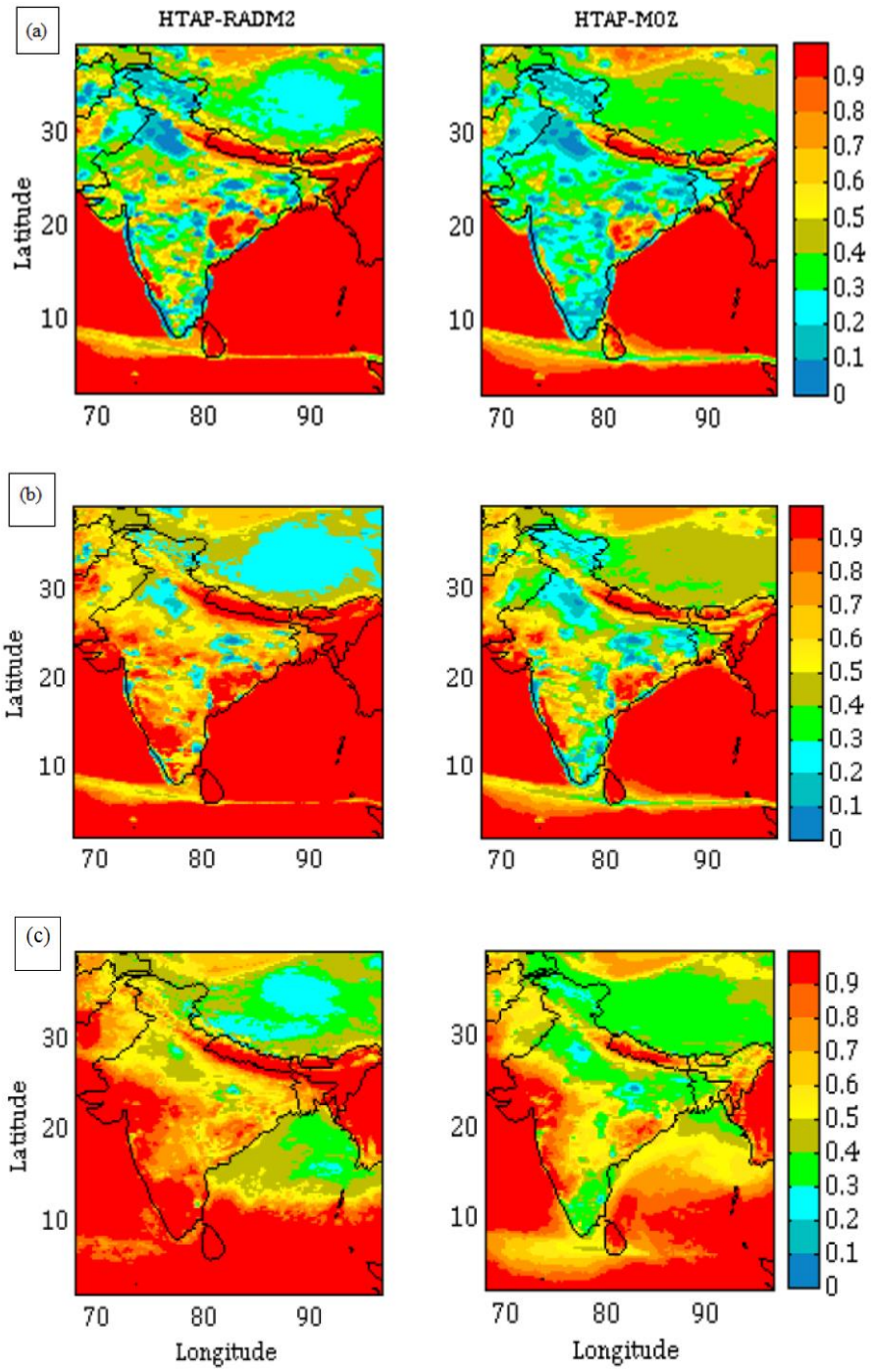

Figure S11. Spatial distribution of daytime (0630-1230 IST) average CH_2O/NO_y ratio comparing simulations with the MOZART and RADM2 chemical mechanisms at model (a) level 1- surface (b) level 3; and (c) level 6 during April. Note the colour scale difference with respect to Fig. 10 in the manuscript.

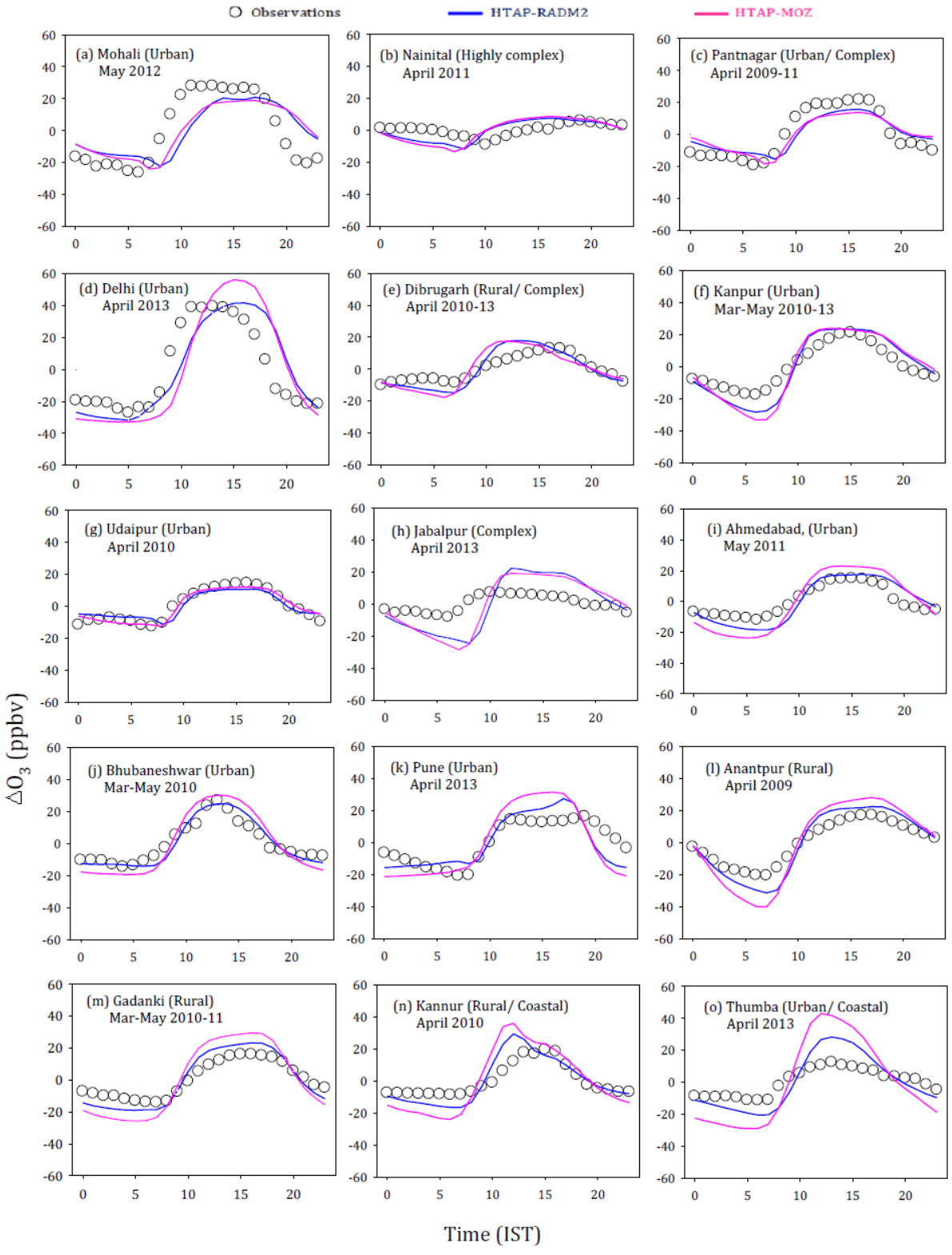

Figure S12. Comparison of monthly average diurnal variation of delta surface ozone (ΔO3), which is the difference between diurnal mean and hourly values, using different chemical mechanisms at various observation sites. Units are in ppbv. Both model simulations are with HTAP emission inventory.

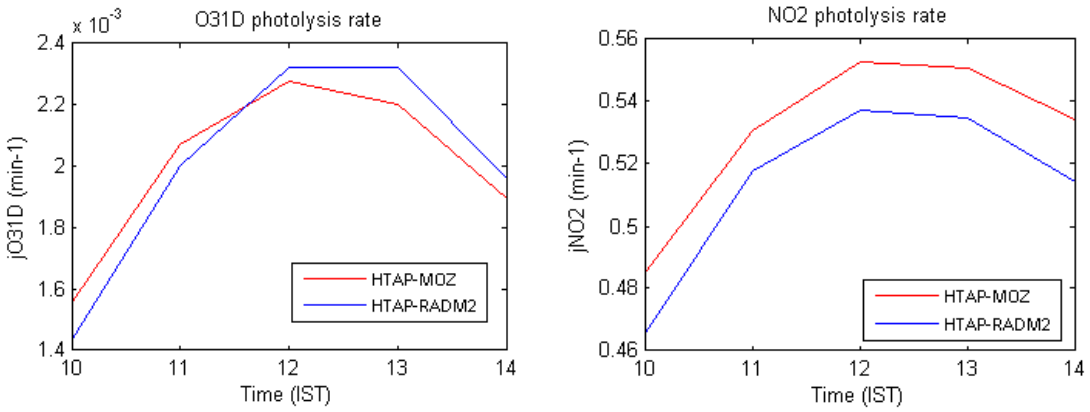

Figure S13. Variation of photolysis rates for O^1D and NO2 from 1000 IST to 1400 IST at surface point in the centre of the domain for 15th April 2013 from HTAP-RADM2 and HTAP-MOZ runs.

References

Gaur, A., Tripathi, S. N., Kanawade, V. P., Tare, V., and Shukla, S. P.: Four-year measurements of trace gases (SO2, NOx , CO, and O3) at an urban location, Kanpur, in Northern India, J. Atmos. Chem., 71, 283–301, 2014.

Renuka, K., Gadhavi, H., Jayaraman, A., Lal, S., Naja, M., and Rao, S.: Study of Ozone and NO2 over Gadanki – a rural site in South India, J. Atmos. Chem., 71, 95–112, doi:10.1007/s10874-014-9284-y, 2014.

Sarangi, T., Naja, M., Ojha, N., Kumar, R., Lal, S., Venkataramani, S., Kumar, A., Sagar, R., and Chandola, H. C.: First simultaneous measurements of ozone, CO and NOy at a high altitude regional representative site in the central Himalayas, J. Geophys. Res.-Atmos., 119, 1592–1611, doi:10.1002/2013JD020631, 2014.

Sarangi, T., Naja, M., Lal, S., Venkataramani, S., Bhardwaj, P., Ojha, N., Kumar, R., and Chandola, H. C.: First observations of light non-methane hydrocarbons (C2–C5) over a high altitude site in the central Himalayas, Atmos. Environ., 125, 450-460, 2016.

Yadav, R., Sahu, L. K., Jaaffrey, S. N. A., and Beig, G.: Distributions of ozone and related trace gases at an urban site in western India. J. Atmos. Chem. 71, 125–144, 2014.