

Supplementary Materials for the manuscript:

Value-added by high-resolution regional simulations of climate-relevant aerosol properties

P. Crippa¹, R. C. Sullivan², A. Thota³, S. C. Pryor^{2,3}

[1] COMET, School of Civil Engineering and Geosciences, Cassie Building, Newcastle University, Newcastle upon Tyne, NE1 7RU, UK

[2] Department of Earth and Atmospheric Sciences, Bradfield Hall, 306 Tower Road, Cornell University, Ithaca, NY 14853, USA

[3] Pervasive Technology Institute, Indiana University, Bloomington, IN 47405, USA

Table S1. Physical and chemical schemes adopted in the WRF-Chem simulations presented herein.

Simulation settings	Values
Domain size	300 × 300 (60 × 60) grid points
Horizontal resolution	12 km (60 km)
Vertical resolution	32 levels up to 50 hPa
Timestep for physics	72 s (300 s)
Timestep for chemistry	5 s
Physics option	Adopted scheme
Microphysics	WRF Single-Moment 5-class
Longwave Radiation	Rapid Radiative Transfer Model (RRTM)
Shortwave Radiation	Goddard
Surface layer	Monin Obhukov similarity
Land Surface	Noah Land Surface Model
Planetary boundary layer	Mellor-Yamada-Janjich
Cumulus parameterizations	Grell 3
Chemistry option	Adopted scheme
Photolysis	Fast J
Gas-phase chemistry	RADM2
Aerosols	MADE/SORGAM
Anthropogenic emissions	NEI (2005)
Biogenic emissions	Guenther, from USGS land use classification

Table S2. Ratio of spatial variability (i.e. the standard deviation of AOD computed across all grid cells) between AOD at wavelengths (λ) of 470, 550 and 660 nm from MODIS observations mapped at 60 km and WRF-Chem simulations conducted at 60 km resolution (WRF60, shown in the table as -60), at 12 km resolution (WRF12, shown in the table as -12), and from WRF-Chem simulations at 12 km but remapped to 60 km (WRF12-remap, shown in the table as -remap). Given WRF12-remap is obtained by averaging WRF12 when at least half of the 5×5 12 km resolution cells contain valid data, the ratio of standard deviations from WRF60 and WRF12-remap may be computed on slightly different observations and sample size. The yellow shading shows for each month and λ the model with ratio of standard deviations closer to 1.

Month→/ Variable↓	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec
470-12	0.489	0.581	0.382	0.595	0.806	0.802	1.033	1.20	1.935	1.698	0.766	0.457
470-60	0.615	0.717	0.682	0.648	0.556	0.331	0.353	0.291	0.541	0.605	0.562	0.564
470-remap	0.522	0.630	0.380	0.644	0.993	0.791	1.018	1.194	2.079	2.099	0.853	0.512
550-12	0.406	0.475	0.307	0.480	0.630	0.690	0.996	1.106	1.709	1.401	0.663	0.370
550-60	0.578	0.663	0.629	0.624	0.502	0.302	0.327	0.274	0.480	0.525	0.518	0.505
550-remap	0.431	0.503	0.299	0.524	0.764	0.693	0.990	1.110	1.872	1.758	0.745	0.396
660-12	0.401	0.454	0.283	0.462	0.571	0.671	1.004	1.114	1.684	1.343	0.665	0.351
660-60	0.458	0.531	0.497	0.462	0.378	0.214	0.225	0.184	0.328	0.391	0.402	0.405
660-remap	0.342	0.393	0.235	0.391	0.553	0.474	0.676	0.777	1.369	1.331	0.557	0.307

Table S3. Spatial coherence in the identification of hourly precipitation between WRF-Chem at different resolutions relative to MERRA-2. The Hit Rate (*HR*) indicates the probability of correct forecast and is the proportion of cells correctly identified as with precipitation by both WRF-Chem and MERRA-2. The Mean Fractional Bias (MFB) in space is also reported for each month and computed from the hourly precipitation rates. The yellow shading indicates the model resolution with highest HR and lower absolute MFB in each month for precipitation.

Month→/ Metric↓	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec
HR-60	0.344	0.298	0.228	0.122	0.083	0.072	0.057	0.059	0.067	0.078	0.154	0.218
HR-remap	0.698	0.715	0.680	0.539	0.402	0.440	0.479	0.438	0.438	0.454	0.581	0.666
MFB-60	-0.340	-0.347	-0.384	-0.442	-0.462	-0.468	-0.475	-0.474	-0.469	-0.459	-0.423	-0.385
MFB-12	-0.095	-0.068	-0.065	-0.168	-0.273	-0.269	-0.260	-0.274	-0.281	-0.261	-0.170	-0.119

Figure S1. Seasonal mean of hourly temperature at 2 meters [K] from MERRA-2 (first row), WRF60 (second row), and WRF12-remap (third row), for simultaneous data from all three datasets.

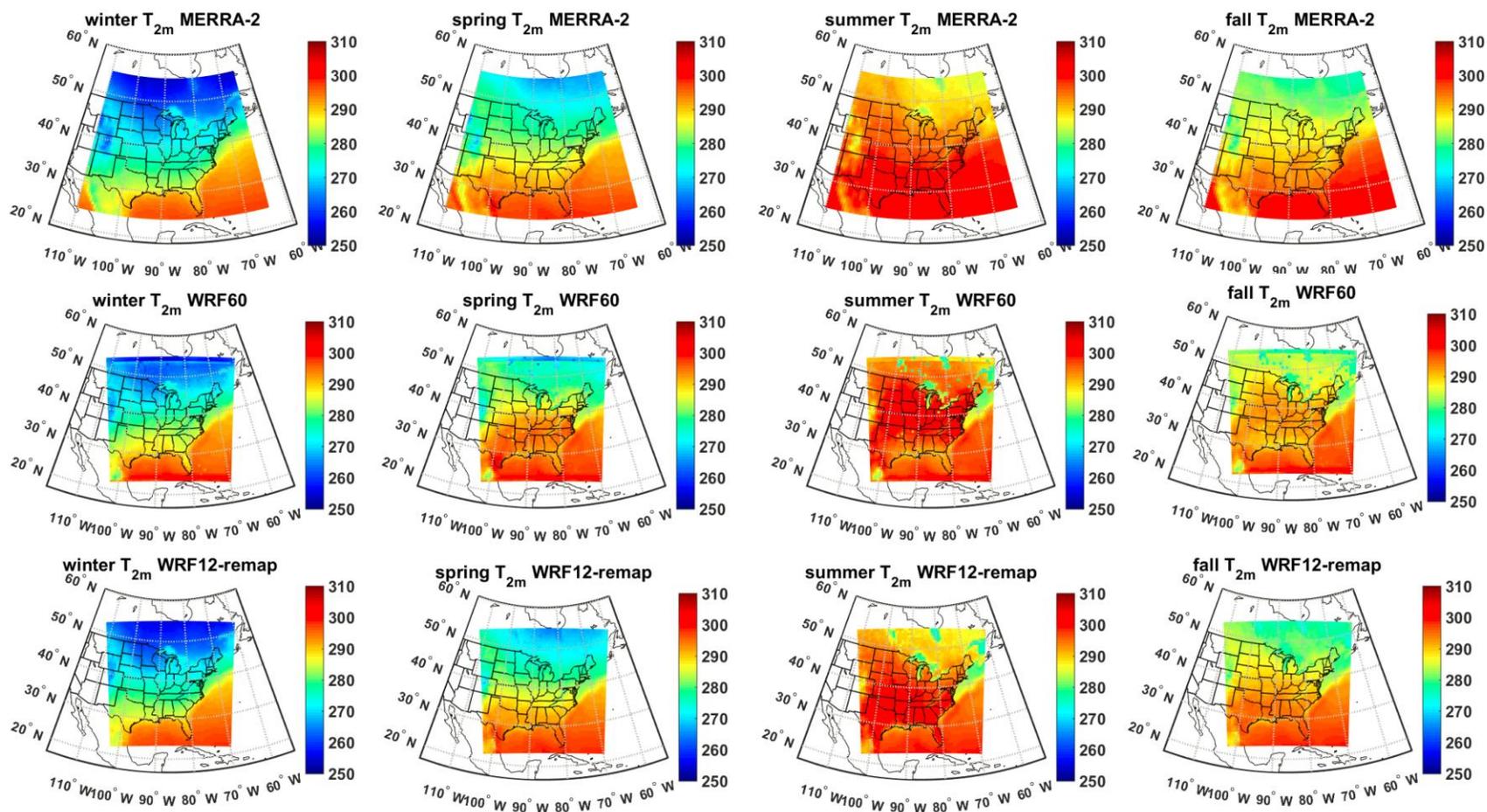


Figure S2. Seasonal average of hourly Planetary Boundary Layer Height, *PBLH* [m] from MERRA-2 (first row), WRF60 (second row), and WRF12-remap (third row), for simultaneous hours of the three datasets.

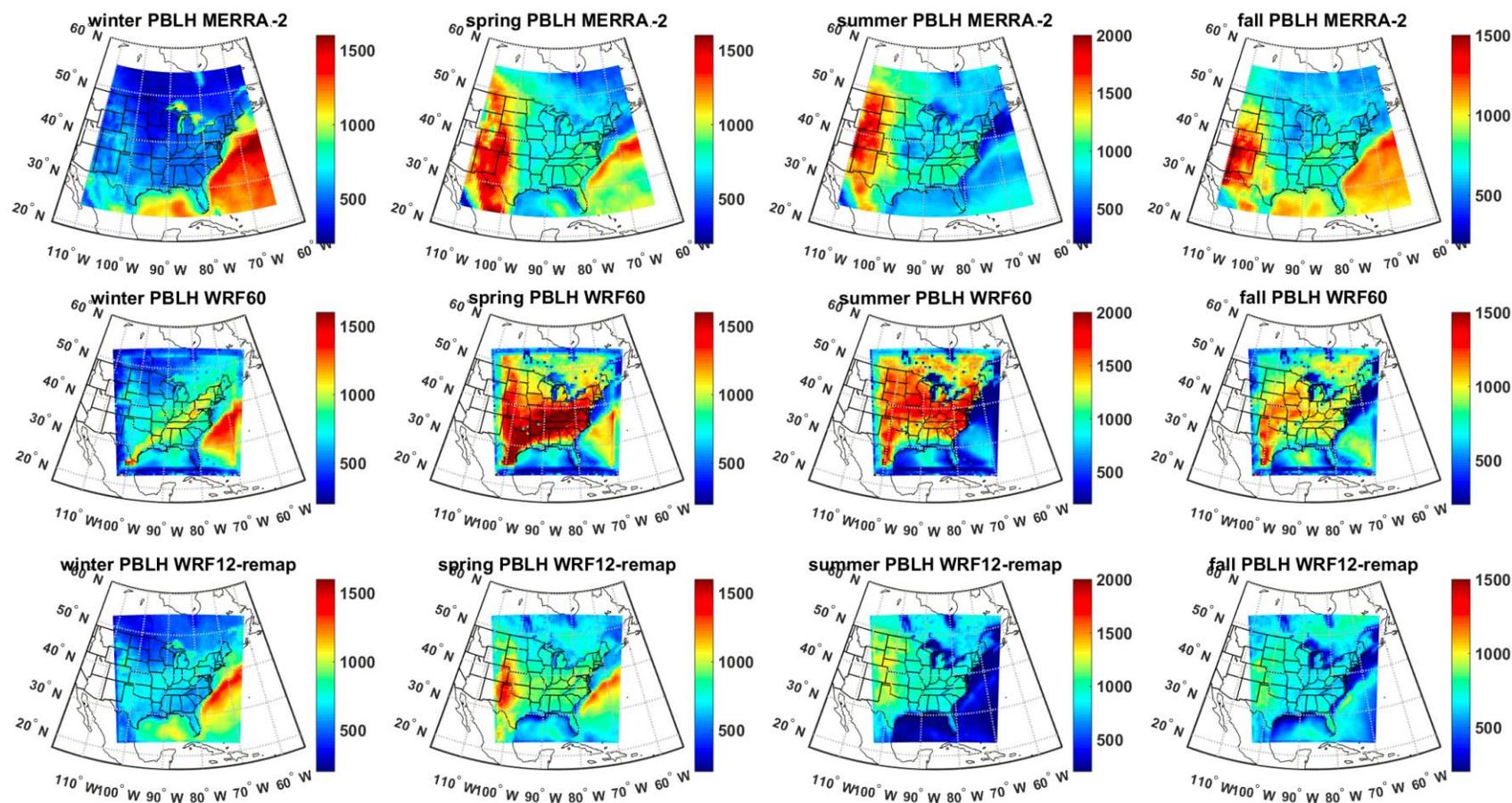


Figure S3. Seasonal total precipitation (mm) from MERRA-2 (first row), WRF60 (second row), and WRF12-remap (third row).

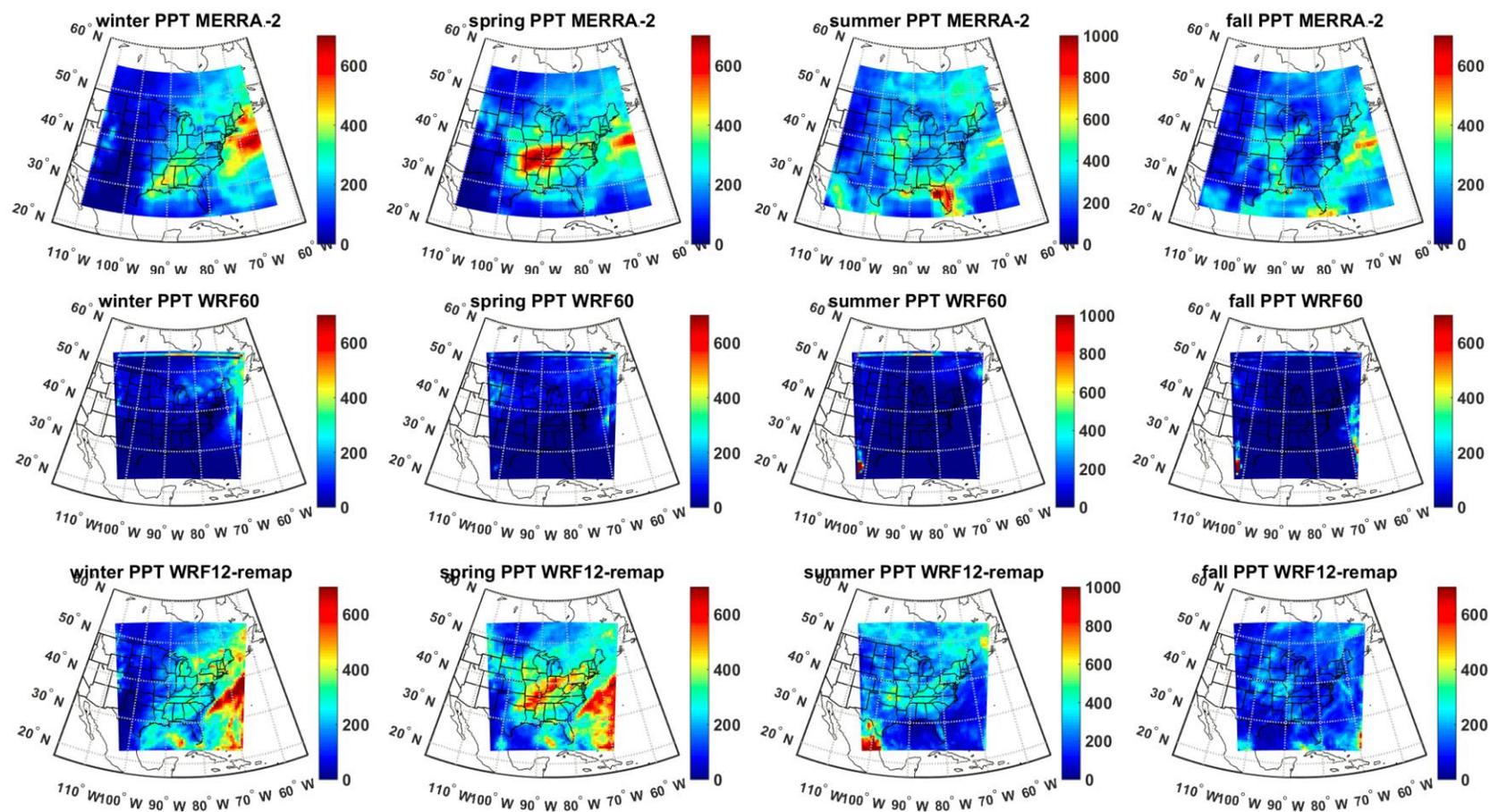


Figure S4. Seasonal total column SO₂ z-scores from OMI (first row), WRF60 (second row), and WRF12-remap (third row). z-scores are computed relative to the spatial seasonal mean of each dataset and indicate the distance from the mean in terms of standard deviation units. A cloud screen of 0.3 is applied to both satellite observations and simulated values. Only grid cells with at least 5 valid observations in a month are used to compute a mean value, otherwise the grid cell is shown as white.

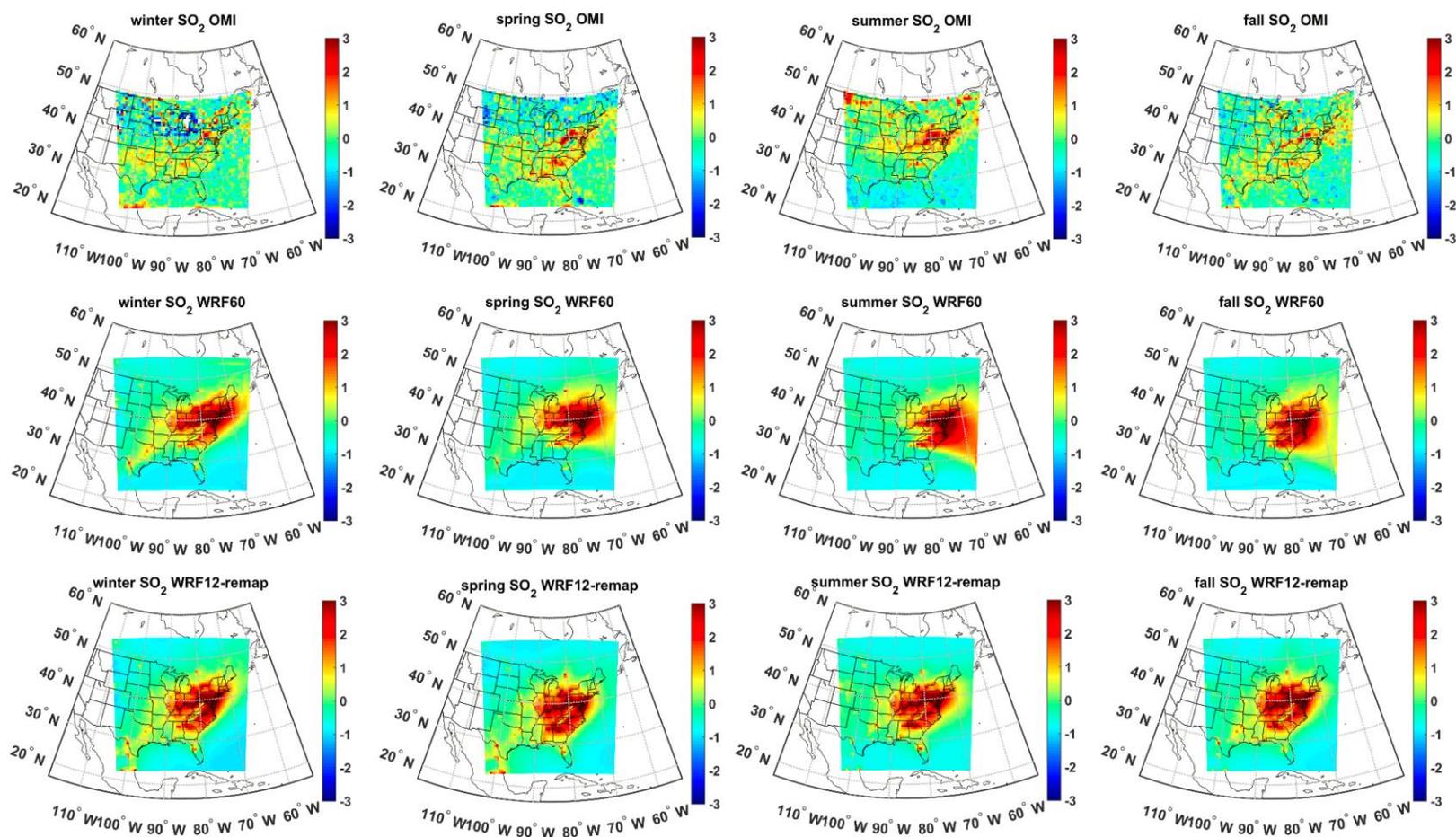


Figure S5. Seasonal total column NO₂ z-scores from OMI (first row), WRF60 (second row), and WRF12-remap (third row). z-scores are computed relative to the spatial seasonal mean of each dataset and indicate the distance from the mean in terms of standard deviation units. A cloud screen of 0.3 is applied to both satellite observations and simulated values. Only grid cells with at least 5 valid observations in a month are used to compute a mean value, otherwise the grid cell is shown as white.

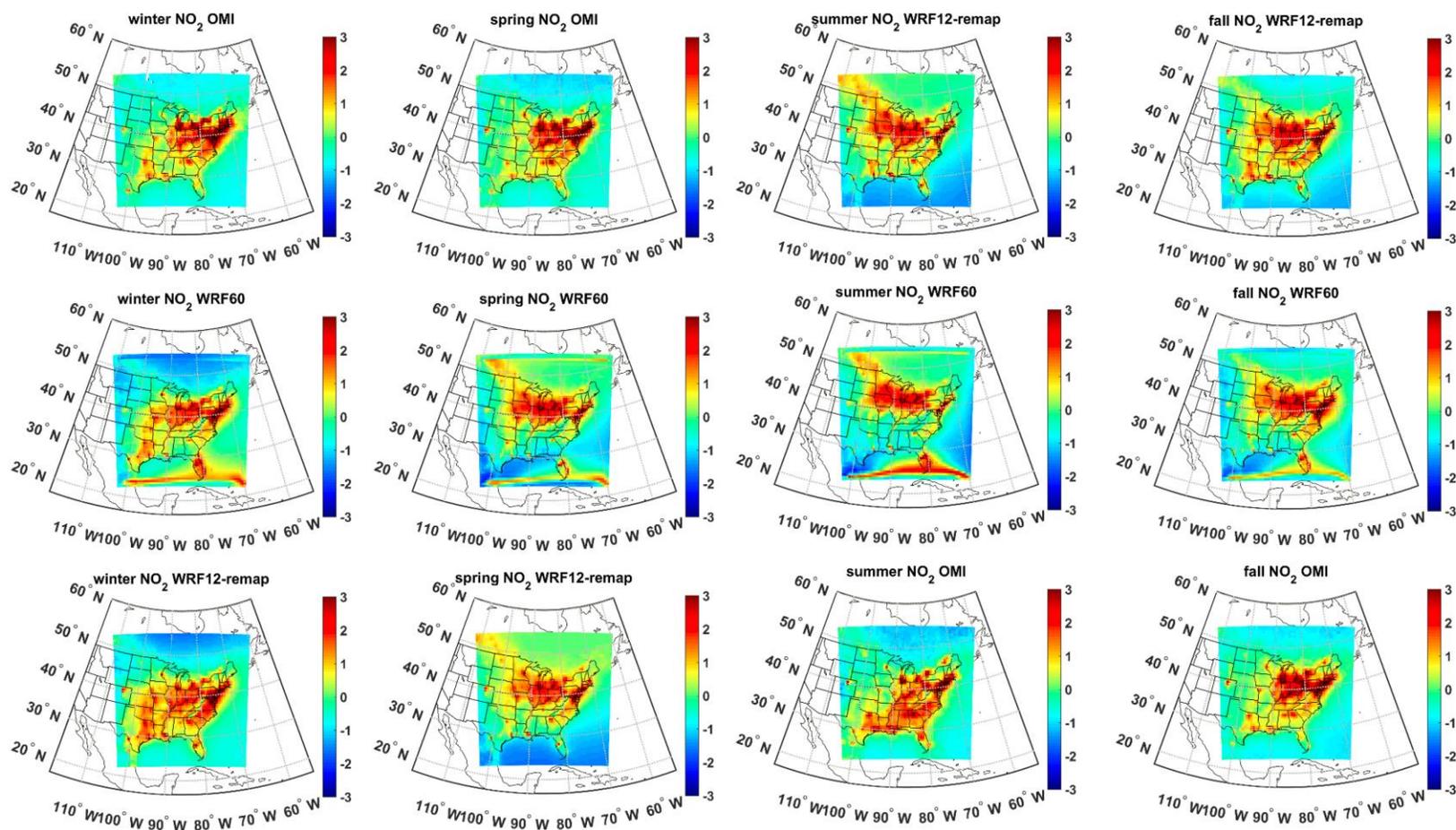


Figure S6. Seasonal total column NH_3 z-scores from OMI (first row), WRF60 (second row), and WRF12-remap (third row). z-scores are computed relative to the spatial seasonal mean of each dataset and indicate the distance from the mean in terms of standard deviation units. A cloud screen of 0.3 is applied to both satellite observations and simulated values. Only grid cells with at least 5 valid observations in a month are used to compute a mean value, otherwise the grid cell is shown as white.

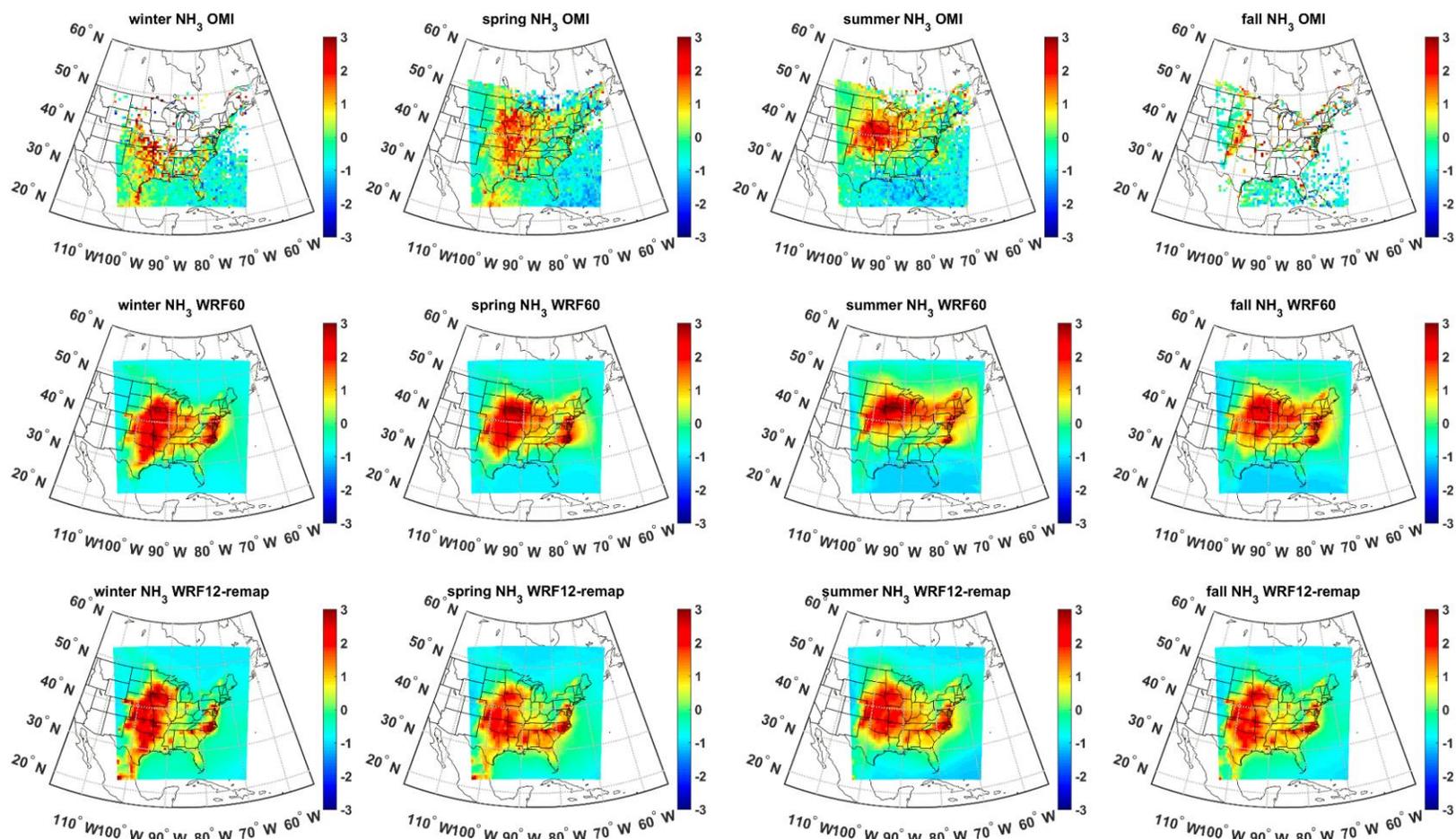


Figure S7. Seasonal total column HCHO z-scores from OMI (first row), WRF60 (second row), and WRF12-remap (third row). z-scores are computed relative to the spatial seasonal mean of each dataset and indicate the distance from the mean in terms of standard deviation units. A cloud screen of 0.3 is applied to both satellite observations and simulated values. Only grid cells with at least 5 valid observations in a month are used to compute a mean value, otherwise the grid cell is shown as white.

