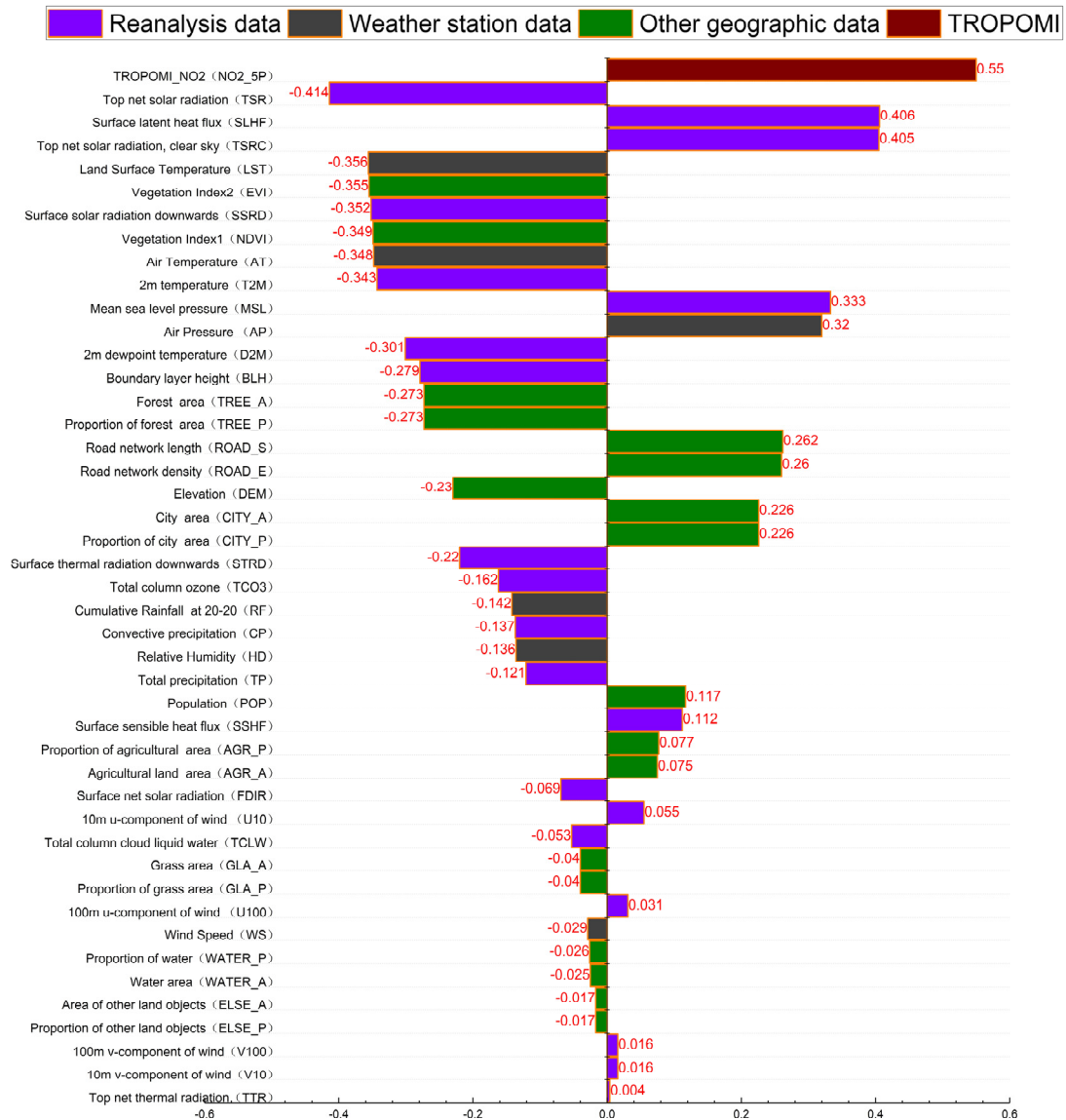


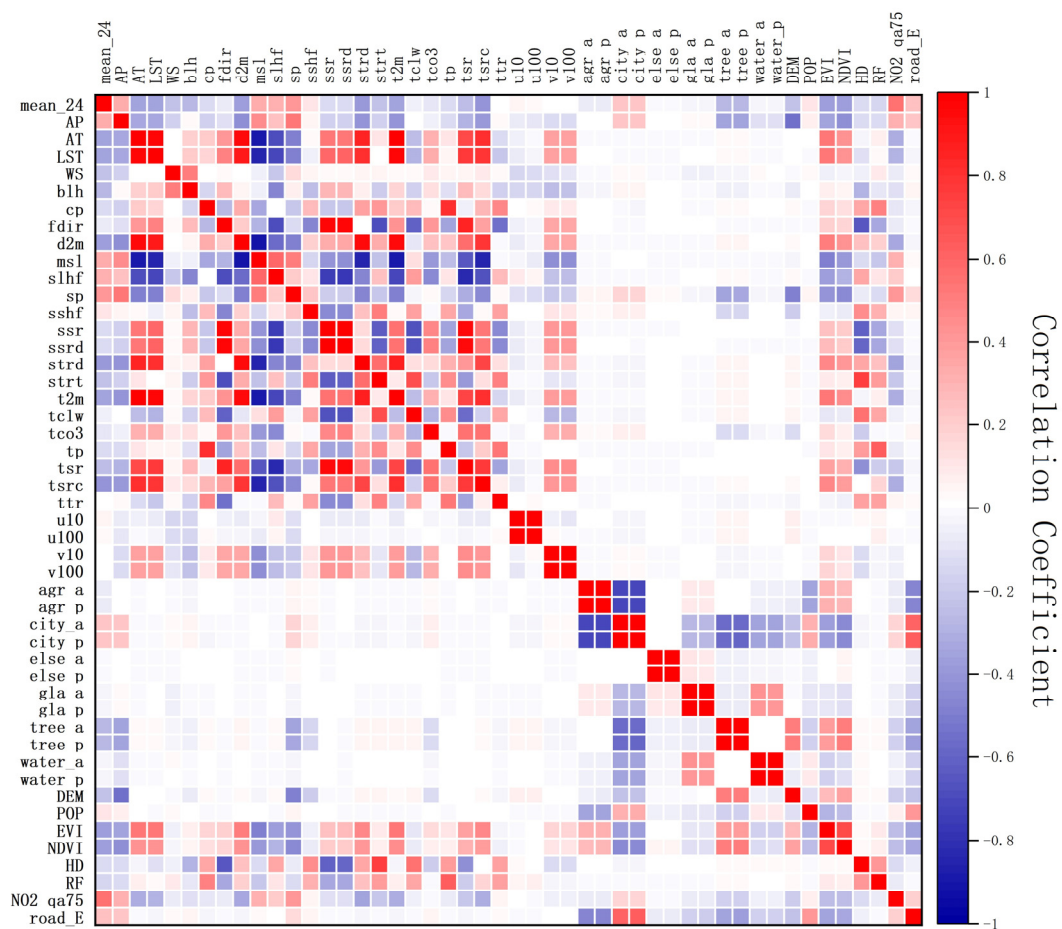
Table S1. Modeling variable preselection table

Variable (abbreviation; unit)	Temporal resolution	Spatial scale	Data source
TROPOMI NO ₂ (NO ₂ _5p; molec/cm ²)	Daily	7 *3.5 km/ 5.5*3.5 km	NASA(National Aeronautics and Space Administration) (https://disc.gsfc.nasa.gov/)
Air Pressure (AP; hPa); Air Temperature (AT; °C); Relative Humidity (HD; %); Land Surface Temperature(LST; °C); Cumulative Rainfall at 20-20(RF; mm); Wind Speed (WS; m/s)	Daily	Station observation ns	National Meteorological Science Data Center (http://data.cma.cn/)
Boundary layer height(BLH; m); Convective precipitation(CP; m); Surface net solar radiation(FDIR; J/m ²); 2m dewpoint temperature(D2M; k); 2m temperature(T2M; k); Mean sea level pressure(MSL; Pa); Surface latent heat flux(SLHF; J/ m ²); Surface pressure(SP; Pa); Surface sensible heat flux(SSHF; J/ m ²); Surface net solar radiation(ssr; J/ m ²); Surface solar radiation downwards(SSRD; J/ m ²); Surface thermal radiation downwards(STRD; J/ m ²); Total column cloud liquid water(TCLW; kg /m ²); Total column ozone(TCO ₃ ; kg /m ²); Total precipitation(TP; m); Top net solar radiation(TSR; J/ m ²); Top net solar radiation, clear sky(TSRC; J/ m ²); Top net thermal radiation(TTR; J/ m ²); 10m u-component of wind(U10; m/s); 100m u-component of wind (U100; m/s); 10m v-component of wind (V10; m/s); 100m v-component of wind (V100; m/s)	1-h	0.25°	European Space Agency, ERA5 (http://maps.elie.ucl.ac.be/CCI/viewer/index.php)
NDVI/EVI	16-day	500m	(Level-1 and Atmosphere Archive and Distribution System,LAADS) https://ladsweb.modaps.eosdis.nasa.gov/search/
Elevation (DEM; m)	-	90m	Shuttle Radar Topography Mission SRTM, https://srtm.csi.cgiar.org/srtmdata/ OpenStreetMap, OSM
Road Network (ROAD)	annual	-	(http://download.geofabrik.de/asia/china.html#)
Population (POP; Peopel)	annual	1km	Worldpop https://www.worldpop.org/
Land Cover (LU)	annual	300m	CCI (Climate Change Initiative) (http://maps.elie.ucl.ac.be/CCI/viewer/index.php)



Pearson Correlation coefficient

(a)



(b)

Figure S1. (a). Pearson correlation between the near-ground NO₂ concentrations and the explanatory variables. (b). Variable correlation heat map.

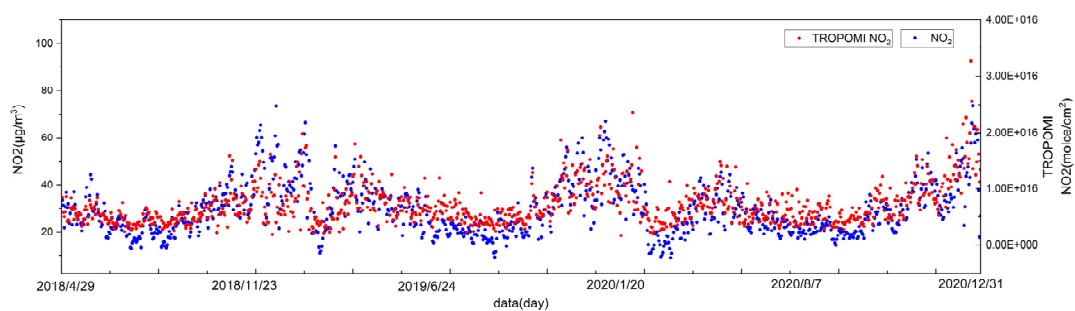


Figure S2. Time variation trend of NO₂ concentrations observed by TROPOMI and ground stations.

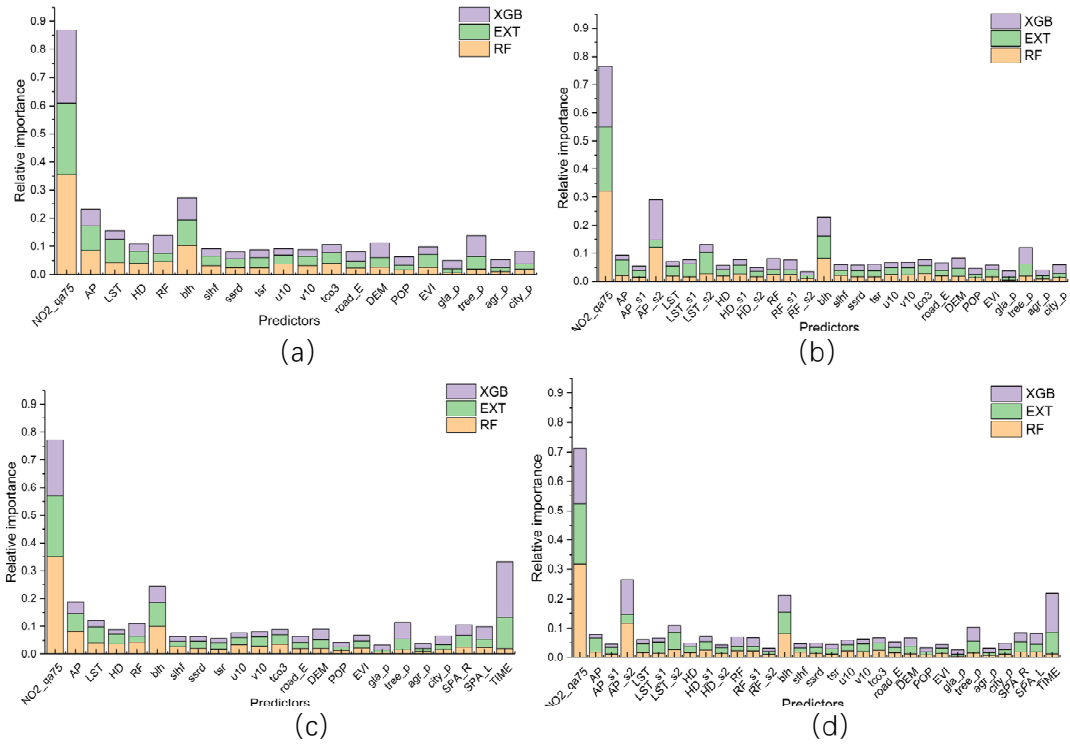


Figure S3. The relative importance of explanatory variables in the three machine learning methods of XGB, EXT and RF: (a) The relative importance of variables in the Plan 1; (b) The relative importance of variables in the Plan 2; (c) The relative importance of variables in the Plan 3; (d) The relative importance of variables in the Plan 4.

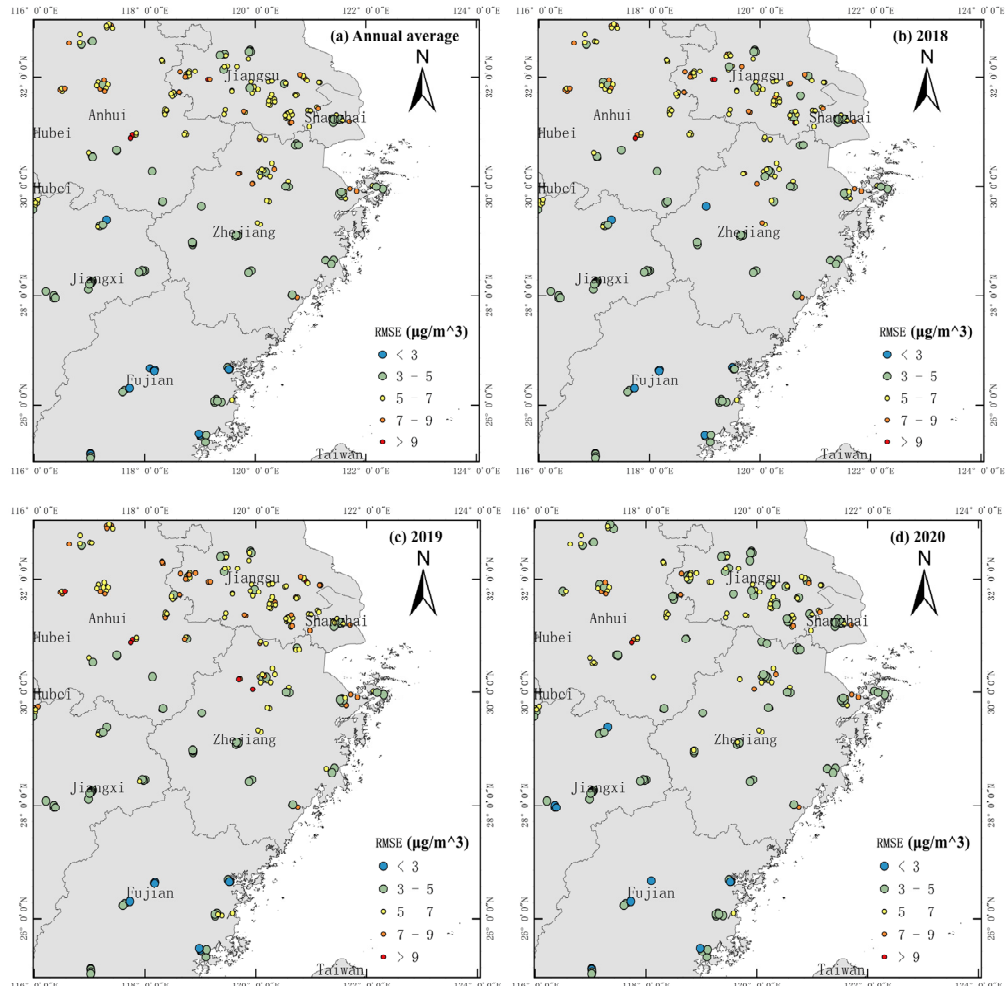


Figure S4. spatial distribution of the local RMSE values of the ensemble model.

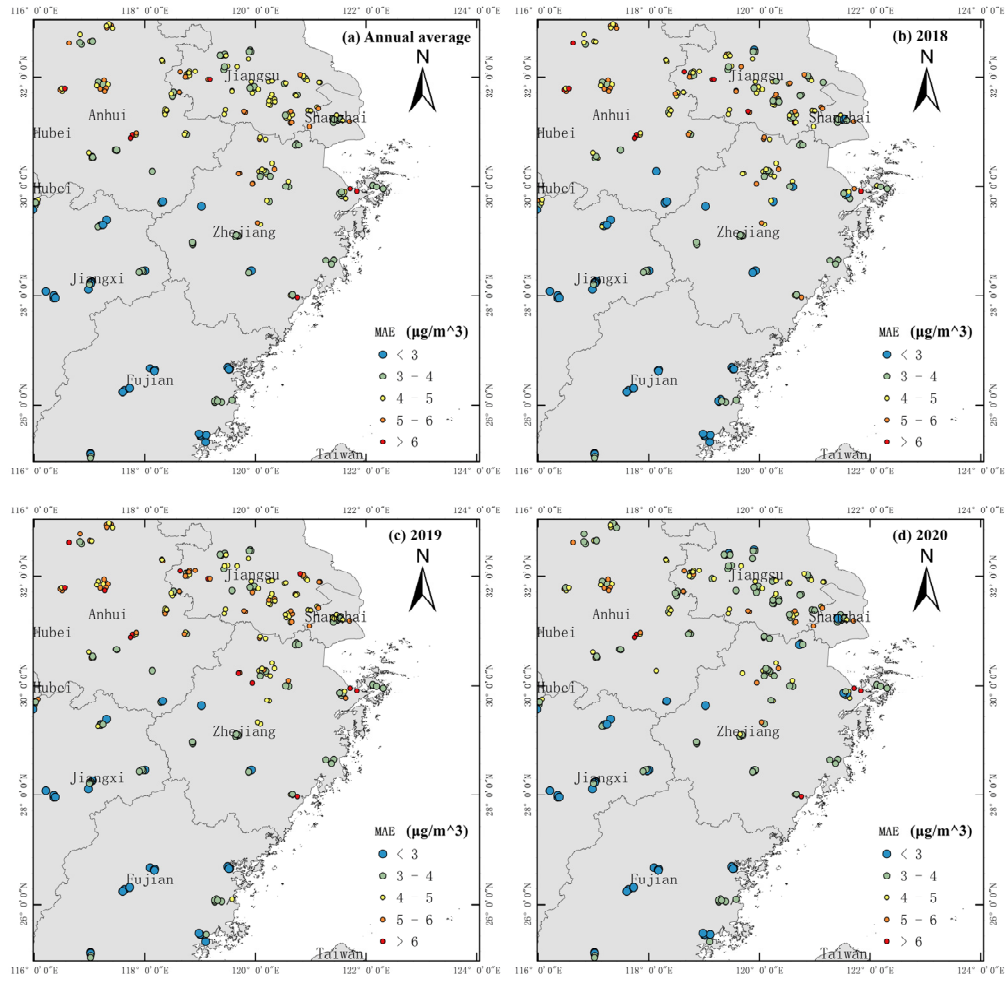


Figure S5. spatial distribution of the local MAE values of the ensemble model.

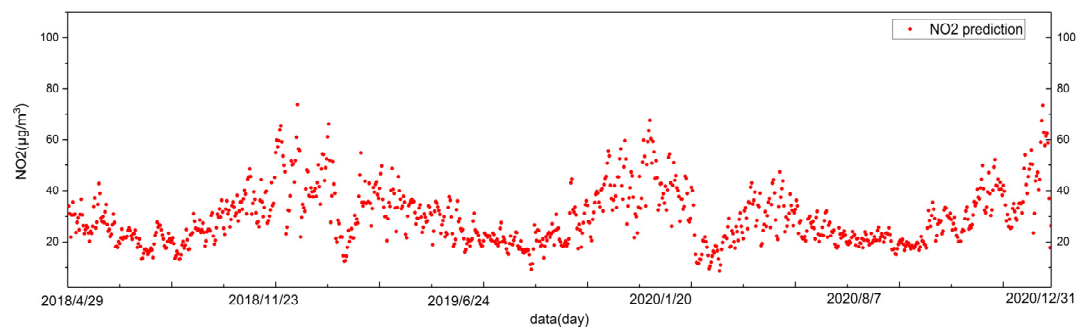


Figure S6. The daily average variation of NO₂ concentrations outputted by the ensemble model.

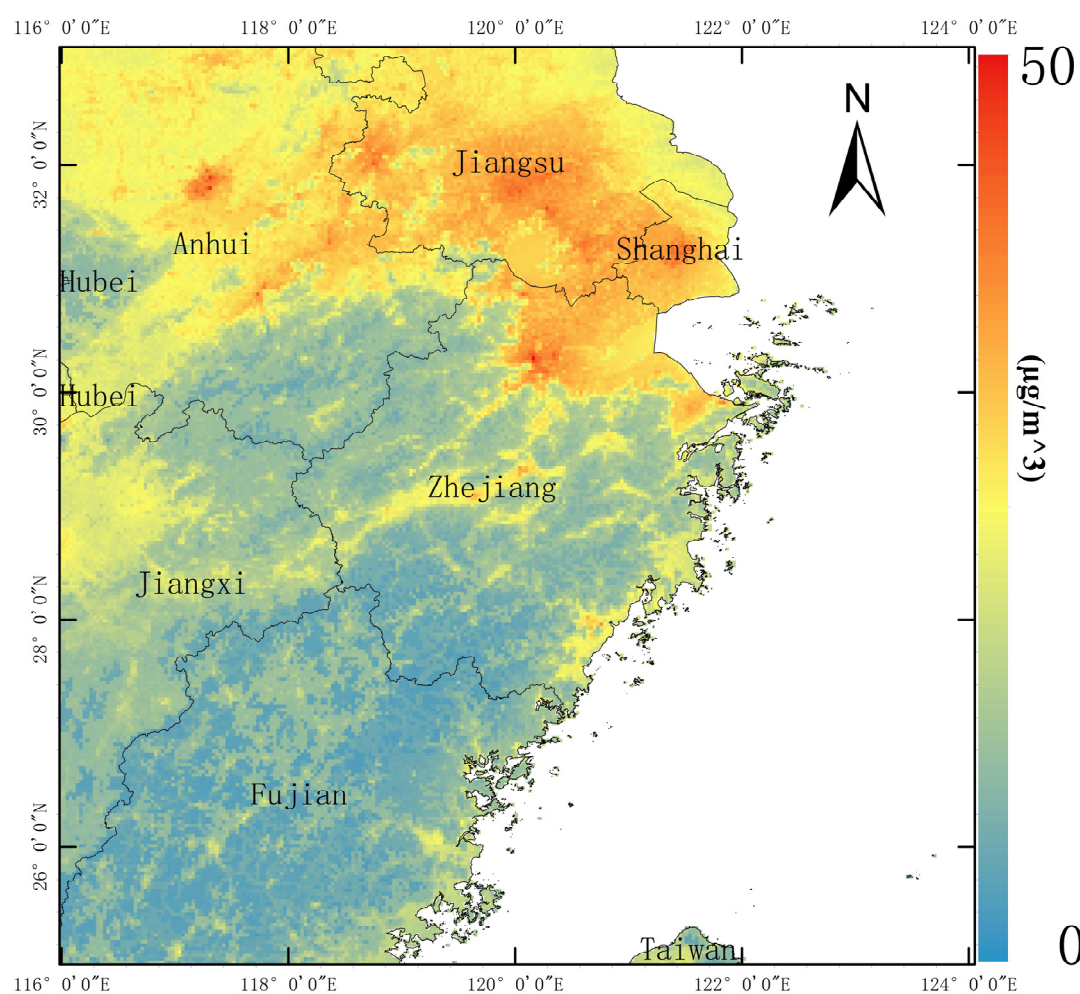


Figure S7. The distribution of the daily average NO₂ concentrations outputted by the ensemble model.

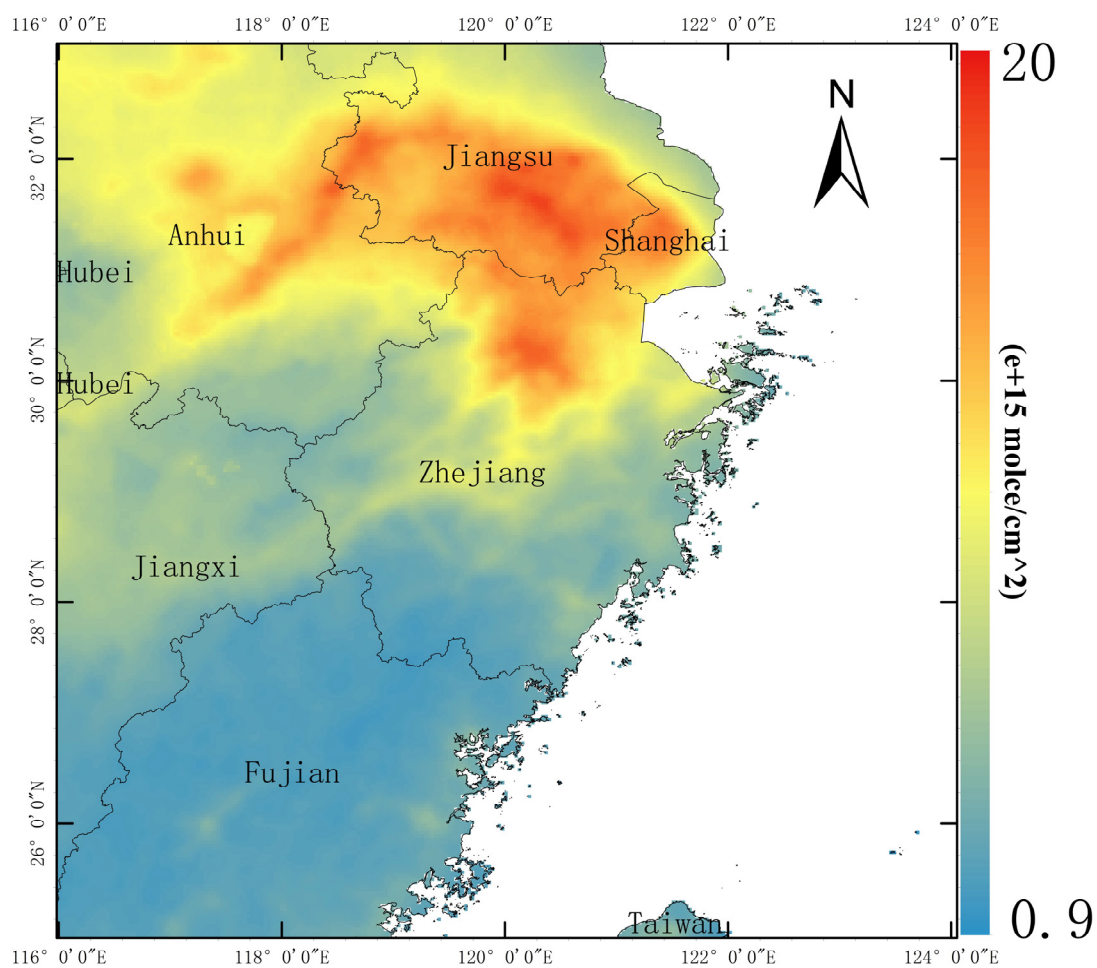


Figure S8. The distribution of daily average tropospheric NO₂ column concentrations interpolated from TROPOMI observations.

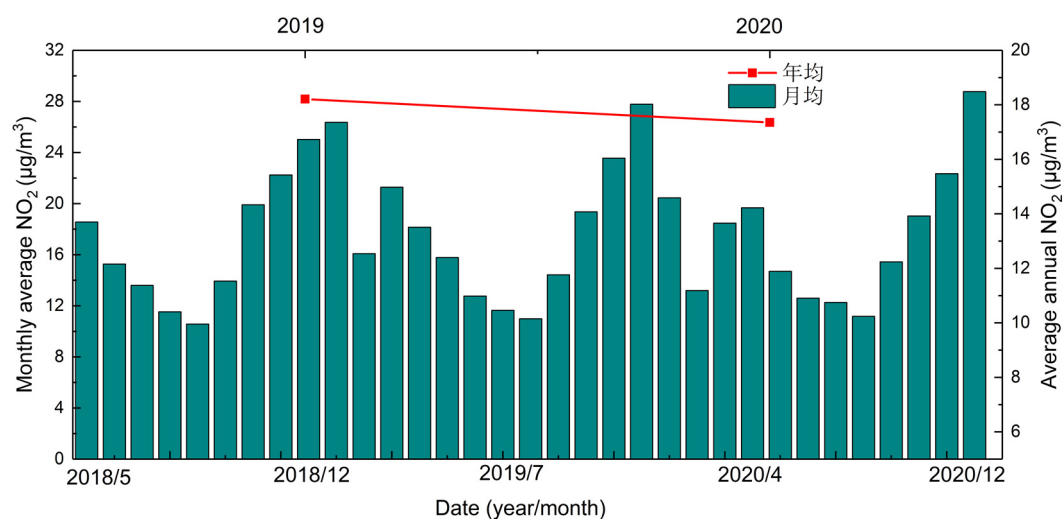


Figure S9. The monthly and annual average variation of NO₂ concentrations outputted by the ensemble model.