1 OMI observations

The NO_2 column concentrations were sourced from NASA Goddard Space Flight Center, specifically from the Goddard Earth Sciences Data and Information Services Center (GES DISC), through the OMI/Aura Multi-wavelength Aerosol Optical Depth and Single Scattering Albedo L3 1-day Best Pixel in 0.25 degree x 0.25 degree V3 (OMAEROe) product (Stein-Zweers and Veefkind, 2012). OMAEROe employs a multi-wavelength algorithm that utilizes up to 20 wavelength bands spanning from 331 nm to 500 nm to select the most accurate aerosol value from Level2G good quality data within each grid. The selection criteria are based on the shortest optical path length, which is determined by the secant of solar zenith angle and secant of viewing zenith angle. We initially processed the daily cloud-screened column amount of NO_2 into monthly OMI column NO_2 data, followed by regridding it to a resolution of 0.5 degrees latitude by 0.625 degrees longitude, equivalent to the GEOS-Chem horizontal resolution.

2 Model validation

We conducted model validation using daily model simulations and ground observations from 2015 to 2017. The R^2 values for NO_2 and $PM_{2.5}$ were found to be 0.73 and 0.79, respectively. These results indicate that the model is capable of capturing the time variation in these pollutants to some extent. The NMB values for NO_2 and $PM_{2.5}$ were 57.68% and 20.4%, respectively, indicating that GEOS-Chem underestimates these pollutants compared to observations. Notably, the underestimation of NO_2 is more severe, with its NMB being more than twice that of $PM_{2.5}$.

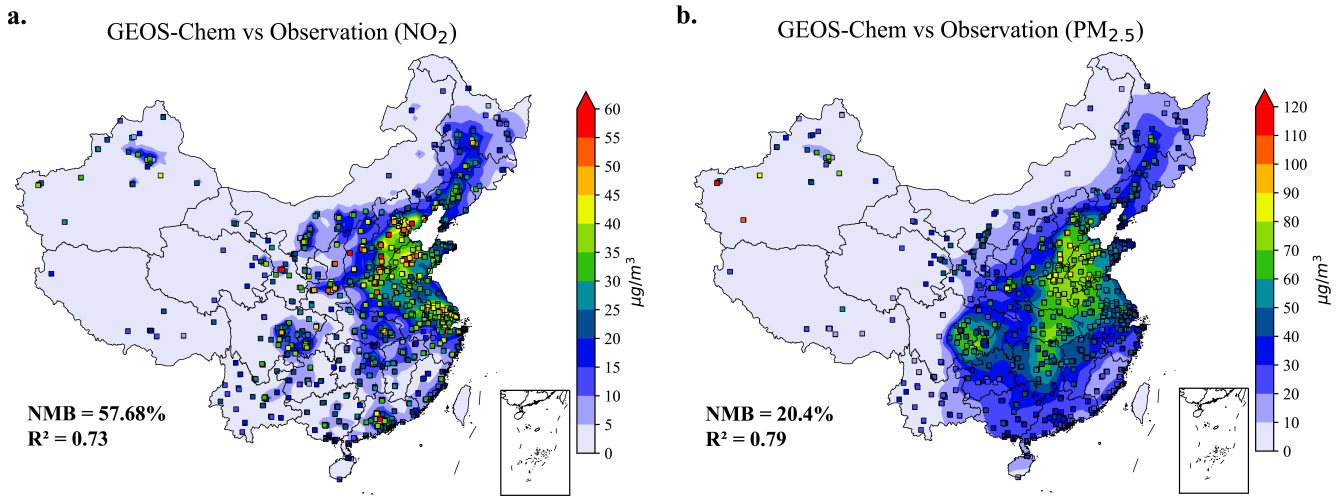

Figure S1. The model validation of GEOS-Chem for the simulation of ground NO_2 and $PM_{2.5}$. Panels a and b denote the three-year averaged ground NO_2 and $PM_{2.5}$ concentrations from GEOS-Chem simulation and ground observations, respectively. The NMB and R^2 for the NO_2 validation is 57.68% and 0.73. The NMB and R^2 for the $PM_{2.5}$ validation is 20.4% and 0.79.

3 Formula of the statistic matrics

$$\mathrm{RMSE} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2} \tag{S1}$$

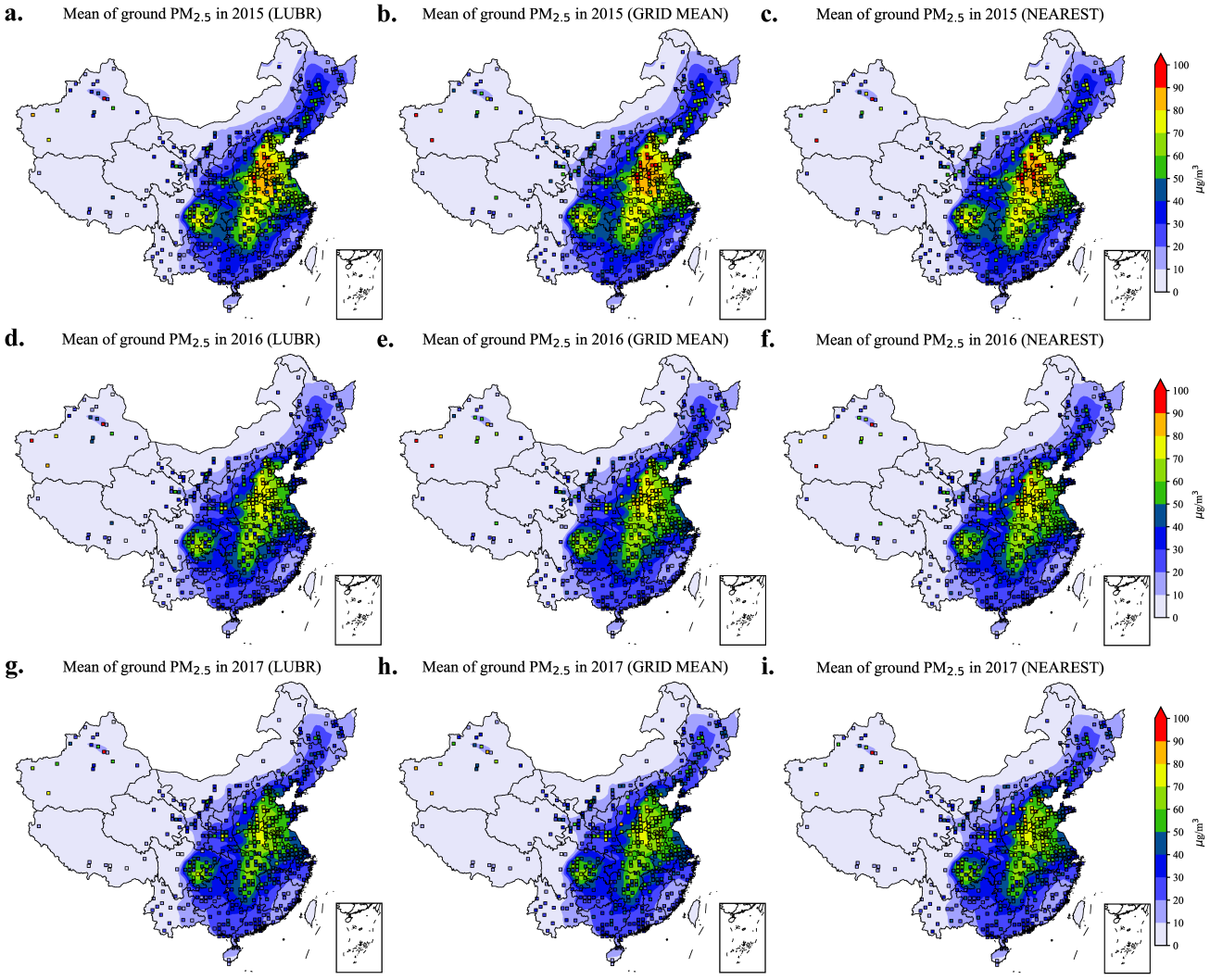

Figure S2. The annual averaged ground $PM_{2.5}$ from GEOS-Chem simulations (filled contours) and the represented observations of simulation grids (colored squares) from three methods. Panels a, d, and g present results using the LUBR method to represent grid $PM_{2.5}$ concentrations for 2015, 2016, and 2017, respectively. Panels b, e, and h present results using the grid mean method. Panels c, f, and i present results using the nearest search method.

$$\text{MAE} = \frac{1}{n}\sum_{i=1}^{n}|y_i - \hat{y}_i| \tag{S2}$$

$$\text{NMB} = \frac{\sum_{i=1}^{n}(y_i - \hat{y}_i)}{\sum_{i=1}^{n}\hat{y}_i} \times 100\% \tag{S3}$$

$$R^2 = 1 - \frac{\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}{\sum_{i=1}^{n}(y_i - \bar{y})^2} \tag{S4}$$

where n represents the size of the dataset, $\hat{y}_i$ and y_i denote the predicted values of GEOS-Chem and true observations, respectively, and $\bar{y}$ represents the mean of the observed values.

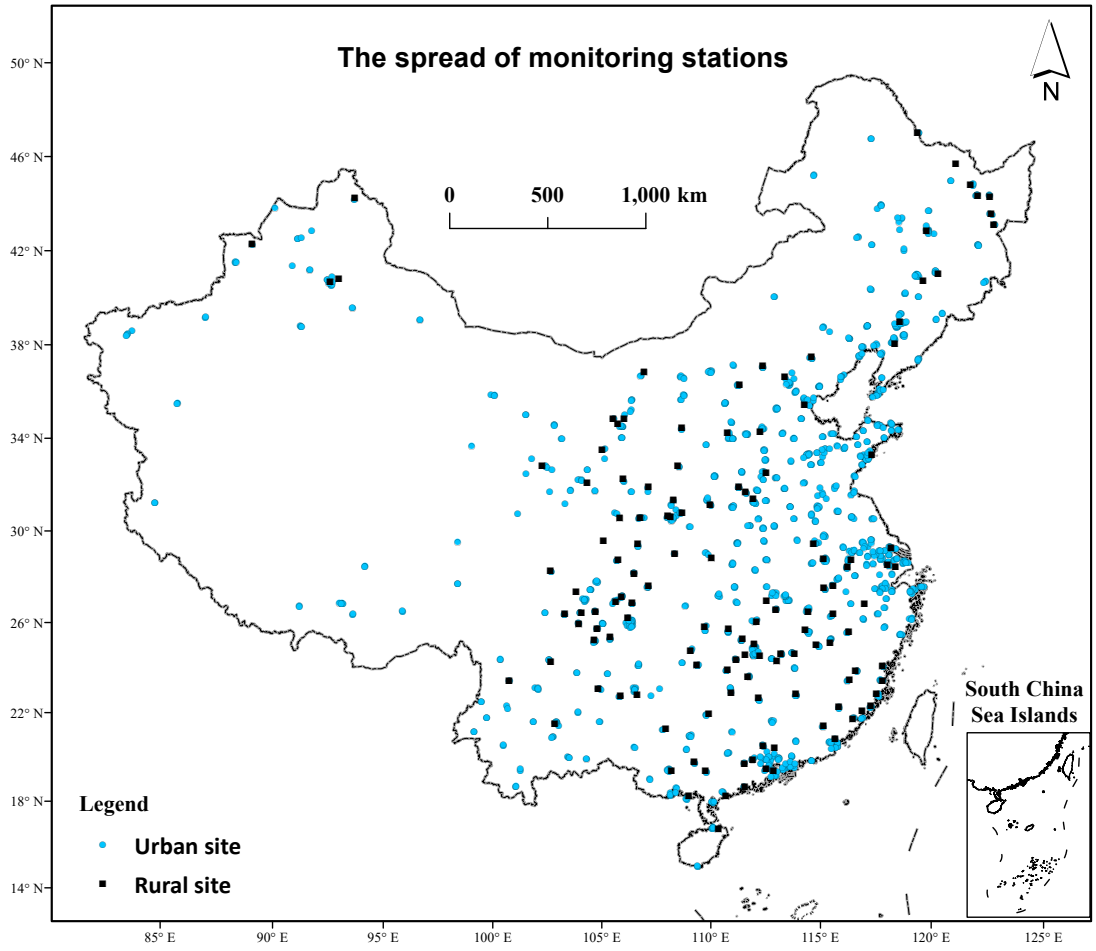

Figure S3. The spread of air quality monitoring stations in China. The turquoise dots and black squares represent urban sites and rural sites, respectively.

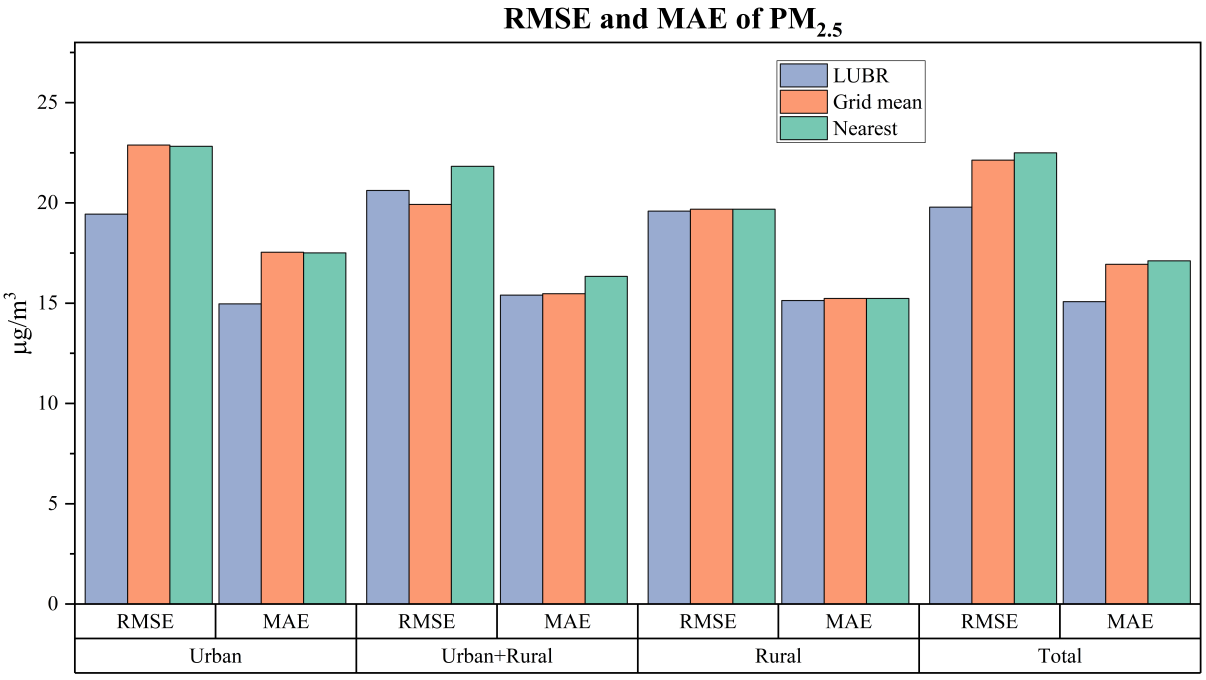

Figure S4. The comprehensive statistical results, encompassing RMSE and MAE, demonstrate the performance of the gridded $PM_{2.5}$ observations compared to the GEOS-Chem simulations. The colors ice blue, rosy red, and cyan represent the LUBR, nearest search, and grid mean methods, respectively. 'Urban,' 'Urban+Rural,' and 'Rural' categorize grids based on the presence of urban and rural sites. 'Urban' includes grids with exclusively urban sites, 'Urban+Rural' includes both urban and rural sites, and 'Rural' comprises grids with only rural sites. 'Total' aggregates results by calculating the average across all three categories.

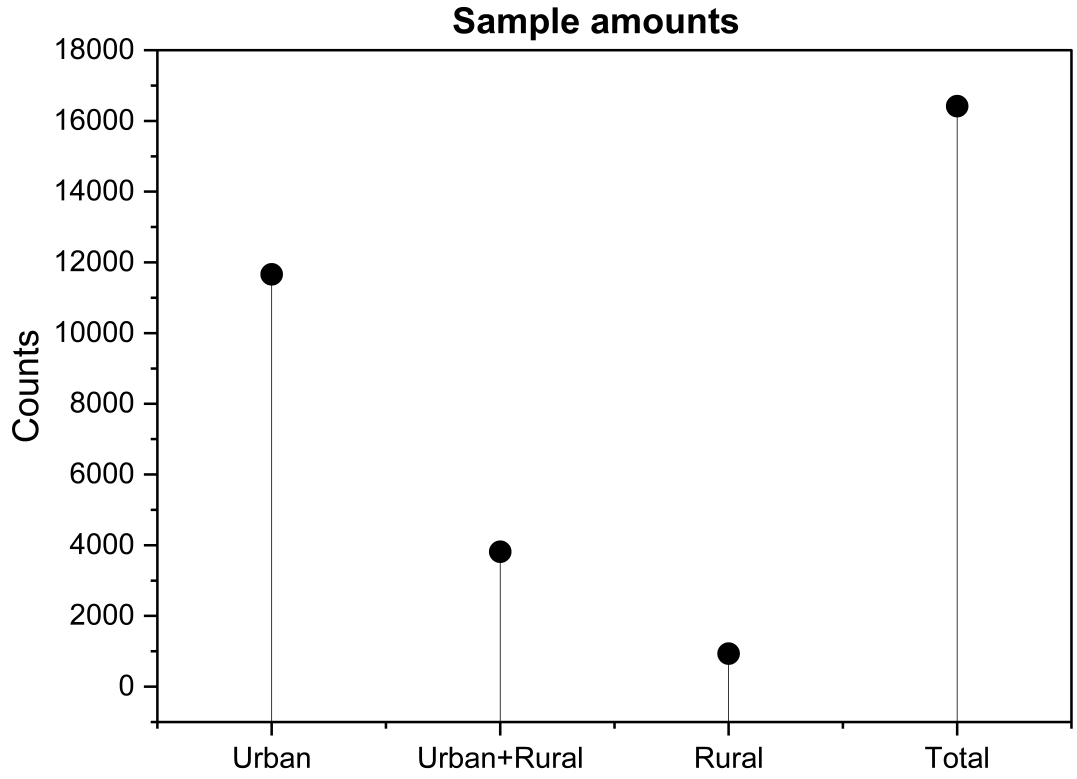

Figure S5. The sample amounts of the categorized grids of ’Urban,’ ’Urban+Rural,’ ’Rural,’ and ’Total’.

References

Stein-Zweers, D. and Veefkind, P.: OMI/Aura Multi-wavelength Aerosol Optical Depth and Single Scattering Albedo L3 1 day Best Pixel in 0.25 degree x 0.25 degree V3, NASA Goddard Space Flight Center, Goddard Earth Sciences Data and Information Services Center (GES DISC), https://doi.org/10.5067/Aura/OMI/DATA3004, last Accessed: 20 Oct 2022, 2012.