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# Supplement of

# A research product for tropospheric $NO_2$ columns from Geostationary Environment Monitoring Spectrometer based on Peking University OMI $NO_2$ algorithm

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#### 1. Derivation of the assumption in the total NO2 SCD correction method

2 In principle, the corrected total NO2 SCDs by combining GEMS and TROPOMI observations

3 should be:

1

4 
$$SCD_{\text{total},h}^{\text{corrected}} = SCD_{\text{total},h}^{\text{GEMS}} + \left(\frac{SCD_{\text{total},h}^{\text{TROPOMI}}}{AMF_{\text{total},h}^{\text{TROPOMI}}} - \frac{SCD_{\text{total},h}^{\text{GEMS}}}{AMF_{\text{total},h}^{\text{GEMS}}}\right) \cdot AMF_{\text{total},h}^{\text{GEMS}}$$

$$= SCD_{\text{total},h}^{\text{TROPOMI}} \cdot \frac{AMF_{\text{total},h}^{\text{GEMS}}}{AMF_{\text{total},h}^{\text{GEMS}}}$$

$$= SCD_{\text{total},h}^{\text{TROPOMI}} \cdot \frac{AMF_{\text{total},h}^{\text{GEMS}}}{AMF_{\text{total},h}^{\text{TROPOMI}}}$$

$$= SCD_{\text{total},h}^{\text{TROPOMI}} \cdot \frac{\text{AMFgeo}_{h}^{\text{GEMS}} \int_{0}^{\infty} w_{\text{h}}^{\text{GEMS}}(z)S(z)dz}{\text{AMFgeo}_{h}^{\text{TROPOMI}} \int_{0}^{\infty} w_{\text{h}}^{\text{TROPOMI}}(z)S(z)dz}$$

$$7 \qquad = \text{SCD}_{\text{total},h}^{\text{TROPOMI}} \cdot \frac{\text{AMFgeo}_{h}^{\text{GEMS}} \left( \int_{z_{\text{T}}}^{\infty} w_{h}^{\text{GEMS}}(z) S(z) dz + \int_{0}^{z_{\text{T}}} w_{h}^{\text{GEMS}}(z) S(z) dz \right)}{\text{AMFgeo}_{h}^{\text{TROPOMI}} \left( \int_{z_{\text{T}}}^{\infty} w_{h}^{\text{TROPOMI}}(z) S(z) dz + \int_{0}^{z_{\text{T}}} w_{h}^{\text{TROPOMI}}(z) S(z) dz \right)}$$

8 
$$\approx \text{SCD}_{\text{total},h}^{\text{TROPOMI}} \cdot \frac{\text{AMFgeo}_{h}^{\text{GEMS}} \left(1 + \int_{0}^{z_{\text{T}}} w_{h}^{\text{GEMS}}(z) S(z) dz\right)}{\text{AMFgeo}_{h}^{\text{TROPOMI}} \left(1 + \int_{0}^{z_{\text{T}}} w_{h}^{\text{TROPOMI}}(z) S(z) dz\right)}$$

9 
$$= SCD_{total,h}^{TROPOMI} \cdot \frac{AMFgeo_h^{GEMS}}{AMFgeo_h^{TROPOMI}} \cdot \frac{1 + \frac{AMF_h^{GEMS}}{AMFgeo_h^{GEMS}}}{1 + \frac{AMF_h^{TROPOMI}}{AMFgeo_h^{TROPOMI}}}$$

In our actual correction, we define and assume the "approximation ratio" as: 10

$$\frac{1 + \frac{\text{AMF}_{h}^{\text{GEMS}}}{\text{AMFgeo}_{h}^{\text{GEMS}}}}{1 + \frac{\text{AMF}_{h}^{\text{TROPOMI}}}{\text{AMFgeo}_{h}^{\text{TROPOMI}}}} \approx 1$$

12 So that the corrected NO<sub>2</sub> SCDs become:

$$SCD_{\text{total},h}^{\text{corrected}} = SCD_{\text{total},h}^{\text{TROPOMI}} \cdot \frac{AMFgeo_h^{\text{GEMS}}}{AMFgeo_h^{\text{TROPOMI}}}$$

- Figure S2 shows the spatial distribution of mean "approximation ratio" in June 2021 which we 14
- assume to be 1. The "approximation ratio" is in the range of 0.9 1.1 in most central and eastern parts 15
- 16 of GEMS FOV, but is smaller in the western and northwestern parts (around 0.8 in most places, with a
- 17 minimum value around 0.7).

18

#### 2. MAX-DOAS instruments

- 19 There are four instruments installed in various areas of Shanghai. The instrument located in the
- 20 campus of Fudan University is in the urban center of Shanghai (31.34°N, 121.52°E). The telescope's

21 azimuth angle is 0°, and the scattered sunlight is measured at ten elevation angles of 2°, 3°, 5°, 7°, 10°, 22 15°, 20°, 30°, 45° and 90° within 15 minutes. The Nanhui site is in the suburban area (31.06°N, 121.80°E) 23 and about 10 km southeast to the center of Shanghai. The azimuth angle is set to 2° and it takes about 15 24 minutes for a full cycle with elevation angles of 2°, 3°, 5°, 7°, 9°, 12°, 15°, 20°, 30°, 45° and 90°. The Dianshan Lake site is located near the Dianshan Lake Scenic Area (31.10°N, 120.98°E), which is at the 25 26 junction of Suzhou and Shanhai. The Chongming site is on the Chongming Island (31.50°N, 121.82°E) 27 of Shanghai, which is China's third largest island and located in Yangtze River estuary. The instruments 28 at Dianshan Lake (suburban) and Chongming (rural) sites are operated in the same way as that in the 29 Nanhui site, except with a fixed azimuth angle at 5° (Zhang et al., 2021; Zhang et al., 2022a; Zhang et 30 al., 2022b; Zhu et al., 2022). 31 The instrument operated in Xianghe is designed by BIRA-IASB and run by both BIRA-IASB and 32 CAS-IAP. It is located in the suburban area (39.75°N, 116.96°E) of Xianghe county to the southwest of 33 Beijing. The telescope's azimuth direction is fixed to the north, and a full scan requiring about 15 minutes comprises nine elevation angles: 2°, 4°, 6°, 8°, 10°, 12°, 15°, 30° and 90°(Clémer et al., 2010; Hendrick 34 35 et al., 2014). 36 The instrument in Xuzhou is set on the roof of the School of Environmental Science and Spatial 37 Informatics, China University of Mining and Technology (34.22°N, 117.14°E). It is located 6.5 km away 38 from the urban center of Xuzhou, and about 1 km south to the Yunlong Lake Scenic Area, which is a 5A 39 natural scenic area. It measures scattered sunlight every 5 minutes for five zenith angles: 5°, 10°, 20°, 40 30° and 90°. This instrument is normally operated from 9:00 to 17:00 local solar time (LST) each day 41 (Liu et al., 2020). 42 The instrument in Hefei site was deployed in March 2008 and is run by Anhui Institute of Optics 43 and Fine Mechanics (AIOFM), Chinese Academy of Science (CAS). It is located outdoors in the campus 44 of AIOFM and about 10 km northwest to the center of Hefei city (31.91°N, 117.16°E). It takes 30 minutes 45 for a cycle to measure introduced scattered sunlight with sequential elevation angles of 3°, 5°, 10°, 20°, 46 30° and 90° (Kanaya et al., 2014). 47 The Fukue and Cape Hedo sites are both remote sites located far away from the major cities 48 (32.75°N, 128.68°E and 26.87°N, 128.25°E, respectively). They are suitable for monitoring tropospheric 49 NO2 in the background regions and outflow from Korea and China. Similar to the instrument at Hefei,

the scattered sunlight is measured by rotating a prism at six elevation angles 3°, 5°, 10°, 20°, 30° and 90°, with 5 minutes for each angle and 30 minutes for a total (Kanaya et al., 2014; Choi et al., 2021).

# 3. Discussion of the differences between POMINO-GEMS and POMINO-TROPOMI v1.2.2 tropospheric NO<sub>2</sub> VCDs

The differences between POMINO-GEMS and POMINO-TROPOMI v1.2.2 tropospheric NO<sub>2</sub> VCDs are related to tropospheric NO<sub>2</sub> AMFs and SCDs. As shown in Figure S10, POMINO-GEMS tropospheric NO<sub>2</sub> AMF is larger than POMINO-TROPOMI v1.2.2 in the western part of GEMS FOV, except over major cities such as Urumqi in China and New Delhi in India, but is smaller in most of the eastern part. Such AMF differences can be further separated into differences in geometric AMF and scattering correction factor.

For a certain pixel and time, GEMS and TROPOMI have the same SZA but different VZAs and thus different geometric AMFs. The GEMS geometric AMFs exhibit a circle-like spatial pattern, increasing from less than 3 in the southeast to more than 5 in the northwest of GEMS FOV, corresponding to the increase of VZA. In contrast, the TROPOMI geometric AMFs exhibit a different spatial pattern with values varying from 2 to 3 (Figure S11). As a result, the GEMS geometric AMFs are larger than

The scattering correction factors of POMINO-GEMS and POMINO-TROPOMI v1.2.2 are different as well. POMINO-GEMS explicitly employs CALIOP-corrected aerosol vertical profiles and recalculates cloud fraction and cloud pressure based on continuum reflectances and O<sub>2</sub>-O<sub>2</sub> SCDs from GEMS observations. By comparison, POMINO-TROPOMI v1.2.2 does not use CALIOP observations to constrain aerosol vertical profiles; and it takes the FRESCO-wide cloud pressure data from the official TROPOMI PAL v2.3.1 NO<sub>2</sub> product and re-calculates cloud fraction at 440 nm. Constraint by CALIOP observations results in higher aerosol-concentrated layer heights (Liu et al., 2019), which enhances the "screening" effect on the absorption by NO<sub>2</sub> and leads to lower scattering correction factors over polluted regions such as eastern China (Figure S12). Higher scattering correction factors of POMINO-GEMS occur over remote areas such as the Pacific Ocean.

those of TROPOMI in the northwest and smaller in the southeast of GEMS FOV.

In addition to tropospheric NO<sub>2</sub> AMFs, the differences in tropospheric NO<sub>2</sub> SCDs between POMINO-GEMS and POMINO-TROPOMI v1.2.2 also contribute to their differences in VCDs. In the correction for total NO<sub>2</sub> SCDs, the corrected total GCDs of GEMS are forced to agree with TROPOMI

PAL v2.3.1 GCDs at the overpass time of TROPOMI. Thus, the difference in geometry between GEMS and TROPOMI leads to different total NO<sub>2</sub> SCDs and hence tropospheric SCDs. In Figure S13c and d, the spatial distribution of differences in tropospheric NO<sub>2</sub> SCDs between POMINO-GEMS and POMINO-TROPOMI v1.2.2 shows positive values over northwestern part and negative values over southeastern part of GEMS FOV.

#### 4. Supplemental tables and figures

## Table S1. Basic information of TROPOMI, OMI, GOME-2 and GEMS instruments

Instrument	Spacecraft	Equator crossing time	Spectral range	Nominal spatial resolution	
TROPOMI	Sentinel-5 Precursor (ESA)		270-500 nm;		
		13:30 LT	675-775 nm;	$3.5 \times 7 \text{ km}^2$ (3.5 × 5.5 km² since 6th Aug. 2019)	
			2305-2385 nm		
OMI	EOS-Aura (NASA)	13:45 LT	270-500 nm	$13 \times 24 \text{ km}^2$	
GOME-2	MetOp-A (EUMETSAT)	9:30 LT	240-790 nm	$80\times40~\text{km}^2$	
GEMS	Geostationary Korea		300-500 nm		
	Multi-Purpose Satellite-	128.2°E over the		$7 \times 8 \text{ km}^2 \text{ (gases)};$	
	2B (GK-2B)			$3.5 \times 8 \text{ km}^2 \text{ (aerosols)}$	

Table S2. Specifics for the NO<sub>2</sub> SCD retrieval of TROPOMI PAL v2.3.1 and GEMS v1.0

	operational products		
	TROPOMI PAL v2.3.1	GEMS v1.0	
Type of DOAS fit	Intensity fit	Optical fit	
$\chi^2$ minimization method	Levenberg-Marquardt	Levenberg-Marquardt	
Wavelength range	405-465 nm	432-450 nm	
C-1	$E_{\rm ref}$ from Chance and Kurucz	$E_{\text{ref}}$ from Chance and Kurucz	
Solar reference spectrum	(2010)	(2010)	
NO mofernior and drawn	$\sigma_{NO_2}~$ at 220 K from Vandaele	$\sigma_{NO_2}~$ at 220 K from Vandaele	
NO <sub>2</sub> reference spectrum	et al. (1998)	et al. (1998)	
0	$\sigma_{\rm O_3}$ at 243 K from	$\sigma_{O_3} \;$ from 243 and 293 K from	
O <sub>3</sub> reference spectrum	Serdyuchenko et al. (2014)	Bogumil et al. (2003)	
0.0	$\sigma_{\rm O_2-O_2}$ at 293 K from	$\sigma_{\rm O_2-O_2}$ at 293 K from	
O <sub>2</sub> -O <sub>2</sub> reference spectrum	Thalman and Volkamer (2013)	Thalman and Volkamer (2013)	
Water vapor reference spectrum	$\sigma_{H_2O_{\text{vap}}}$ at 293 K from	Not yet applied	

#### HITRAN 2012 data

Liquid water reference spectrum	$\sigma_{\rm H_2O_{liq}}$ from Pope and Fry (1997)	Not yet applied	
Ding reference encetrum	$I_{\text{ring}}$ derived following Chance	$\sigma_{ring}$ derived following	
Ring reference spectrum	and Spurr (1997)	Chance and Spurr (1997)	

Table S3. Ground based MAX-DOAS measurements

G'4					
Site name	Type	Geolocation	Measurement time		
For Lor II. 'consul's	Urban	101 500E 21 240N	1 June – 31 August		
Fudan University		121.52°E, 31.34°N	2021		
Xuzhou	Suburban	117.14°E, 34.22°N	1 June – 31 August		
Auzhou	Suburbun	117.14 E, 54.22 1	2021		
Hefei	Suburban	117.16°E, 31.91°N	1 June – 30 June 2021		
Nanhui	Suburban	121 000E 21 060NI	1 June – 31 August		
Namui	Suburban	121.80°E, 31.06°N	2021		
Xianghe	Suburban	116.96°E, 39.75°N	1 June – 31 August		
Alanghe	Suburban	110.90 E, 39.73 N	2021		
Dianshan Lake	Suburban	120.98°E, 31.30°N	1 June – 31 August		
Diansnan Lake	Suburban	120.98 E, 31.30 N	2021		
Ch an amin a	Rural	121.82°E, 31.50°N	1 June – 31 August		
Chongming	Kurai	121.82 E, 31.30 N	2021		
Fukue	Remote	120 (00E 22.75°N)	1 June – 31 August		
rukue	Remote	128.68°E, 32.75°N	2021		
Constitution	D	100 050E 07 070N	1 June – 31 August		
Cape Hedo	Remote	128.25°E, 26.87°N	2021		

Table S4. Evaluation of surface NO<sub>2</sub> concentrations derived from POMINO-GEMS with total

# SCD correction and POMINO-GEMS without correction using MEE measurements

	POMINO-GEMS		POMINO-GEMS		
MEE sites	with total SCD correction		without tot	without total SCD correction	
	R	NMB	R	NMB	
All	0.97	-34.4%	0.97	-27.1%	
Urban	0.97	-28.7%	0.97	-19.8%	
Suburban	0.97	-42.8%	0.97	-38.0%	
Rural	0.96	-48.4%	0.96	-44.4%	

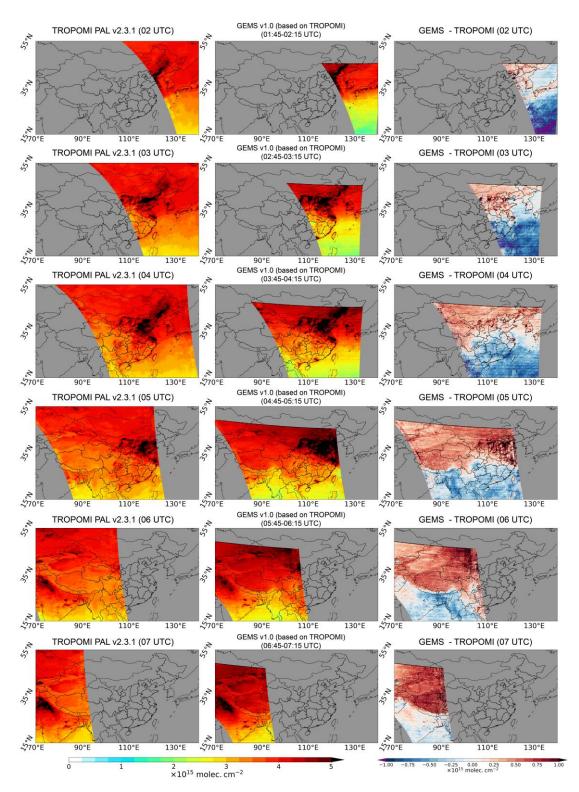


Figure S1. Spatial distribution of monthly mean total  $NO_2$  GCDs at each hour on a  $0.05^\circ \times 0.05^\circ$  grid in June 2021. Left column, TROPOMI PAL v2.3.1 product; middle column, GEMS v1.0 product that spatiotemporally matches with TROPOMI; right column, the absolute differences of GEMS total  $NO_2$  GCDs from those of TROPOMI. The regions in grey mean there are no valid observations.

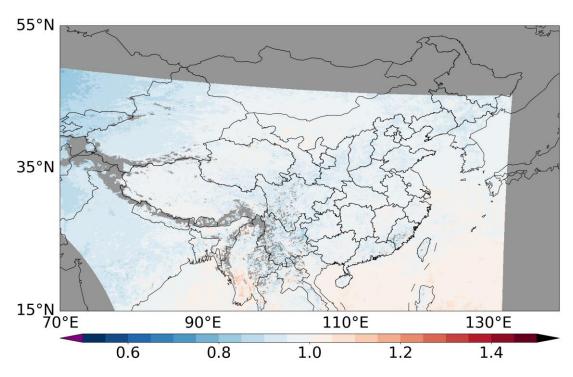


Figure S2. Spatial distribution of mean approximation ratios on a  $0.05^{\circ} \times 0.05^{\circ}$  grid in June 2021. The regions in grey mean there are no valid NO<sub>2</sub> observations.

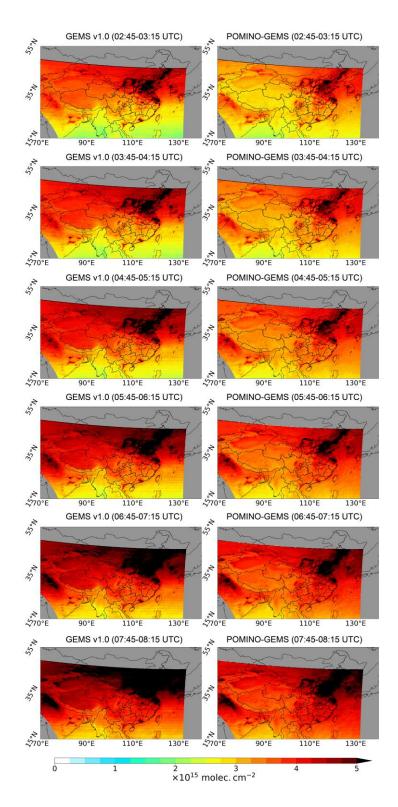


Figure S3. Spatial distribution of monthly mean total  $NO_2$  GCDs at each hour on a  $0.05^\circ \times 0.05^\circ$  grid in June 2021. Left column, official GEMS v1.0 product; right column, corrected POMINO-GEMS product. The regions in grey mean there are no valid observations.

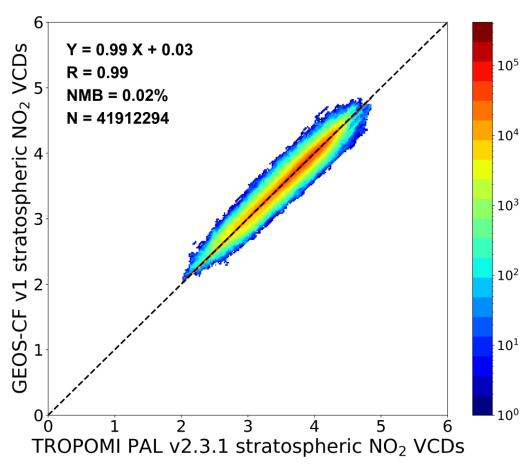


Figure S4. Scatterplot for stratospheric NO<sub>2</sub> VCDs between GEOS-CF v1 and TROPOMI PAL v2.3.1 products in June 2021. Colors represent the data density.

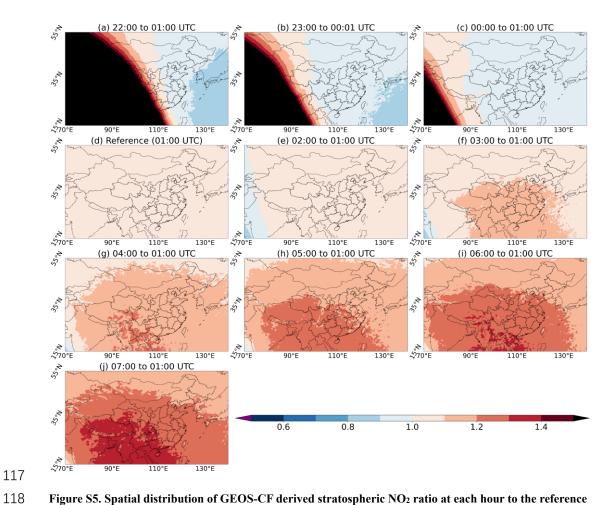


Figure S5. Spatial distribution of GEOS-CF derived stratospheric  $NO_2$  ratio at each hour to the reference hour (01:00 UTC) on a  $0.05^\circ \times 0.05^\circ$  grid in June 2021.

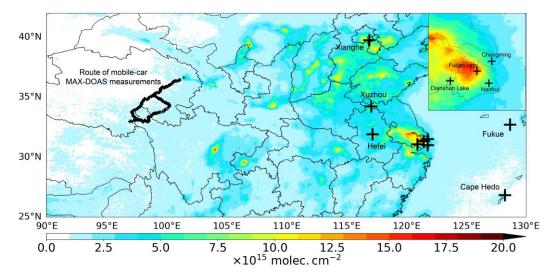


Figure S6. Spatial distribution of ground-based MAX-DOAS sites and the route of mobile-car MAX-DOAS measurements used in this study. Overlaid in the background is the spatial distribution of POMINO-GEMS tropospheric  $NO_2$  VCDs in JJA 2021 on a  $0.05^\circ \times 0.05^\circ$  grid.

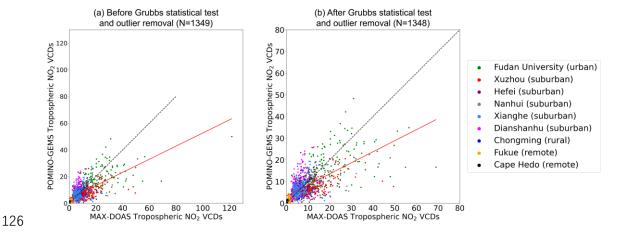


Figure S7. Scatterplots for tropospheric  $NO_2$  VCDs (×  $10^{15}$  molec. cm<sup>-2</sup>) between MAX-DOAS and POMINO-GEMS at all GEMS observation hours in JJA 2021 (a) before and (b) after performing Grubbs statistical test and outlier removal. Only one outlier is identified.

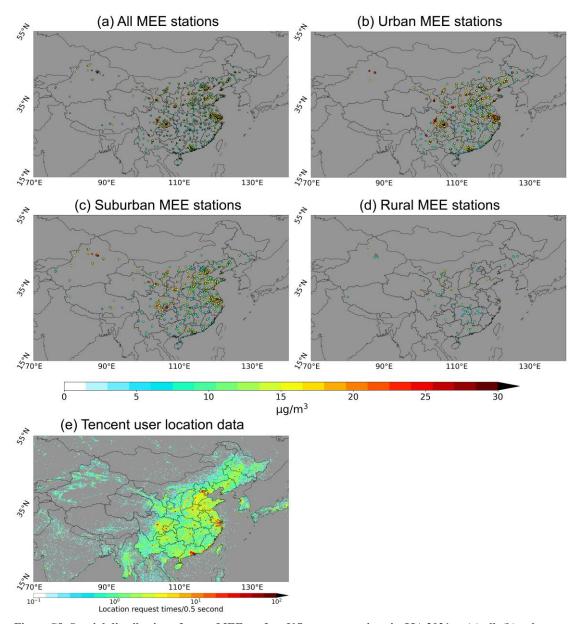


Figure S8. Spatial distribution of mean MEE surface NO<sub>2</sub> concentrations in JJA 2021 at (a) all, (b) urban, (c) suburban and (d) rural sites. The classification is based on (e) mean Tencent user location data from 31 August to 30 September 2021 in China. The regions in grey mean there are no valid observations.

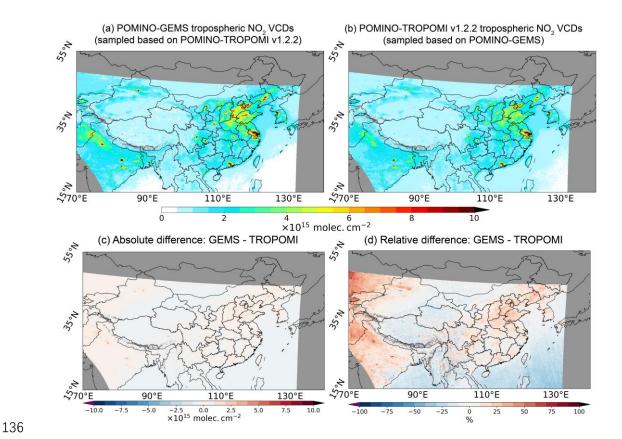


Figure S9. Spatial distribution of (a) POMINO-GEMS and (b) POMINO-TROPOMI v1.2.2 tropospheric NO $_2$  VCDs on a  $0.05^\circ \times 0.05^\circ$  grid in JJA 2021. (c) and (d) are absolute and relative differences of POMINO-GEMS tropospheric NO $_2$  VCDs from those of POMINO-TROPOMI v1.2.2, respectively. Data are sampled from locations and times with valid data in both POMINO-GEMS and POMINO-TROPOMI v1.2.2. The regions in grey mean there are no valid observations.

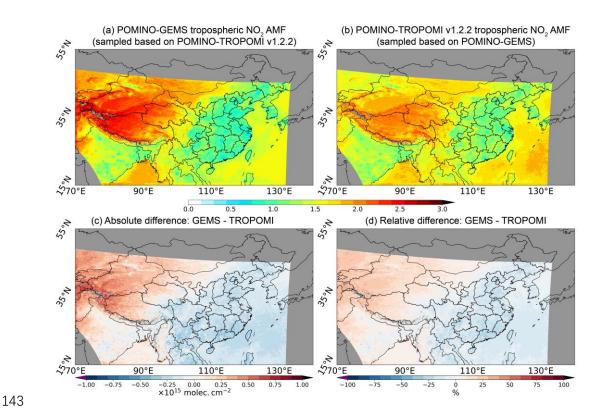


Figure S10. Spatial distribution of (a) POMINO-GEMS and (b) POMINO-TROPOMI v1.2.2 tropospheric NO<sub>2</sub> AMFs on a  $0.05^{\circ} \times 0.05^{\circ}$  grid in JJA 2021. (c) and (d) are absolute and relative differences of POMINO-GEMS tropospheric NO<sub>2</sub> AMFs from those of POMINO-TROPOMI v1.2.2, respectively. Data are sampled from locations and times with valid NO<sub>2</sub> VCD data in both POMINO-GEMS and POMINO-TROPOMI v1.2.2. The regions in grey mean there are no valid NO<sub>2</sub> observations.

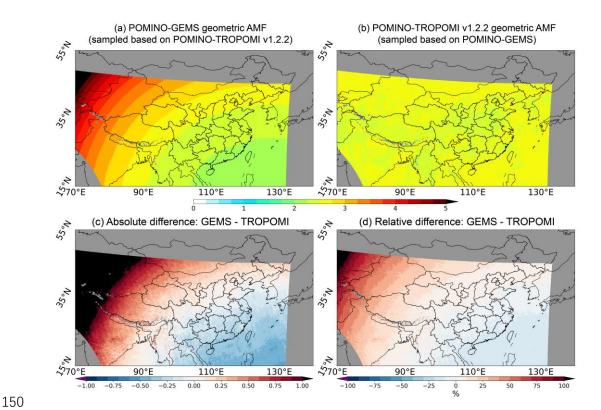


Figure S11. Spatial distribution of (a) POMINO-GEMS and (b) POMINO-TROPOMI v1.2.2 geometric AMFs on a  $0.05^{\circ} \times 0.05^{\circ}$  grid in JJA 2021. (c) and (d) are absolute and relative differences of POMINO-GEMS geometric AMFs from those of POMINO-TROPOMI v1.2.2, respectively. Data are sampled from locations and times with valid NO<sub>2</sub> VCD data in both POMINO-GEMS and POMINO-TROPOMI v1.2.2. The regions in grey mean there are no valid NO<sub>2</sub> observations.

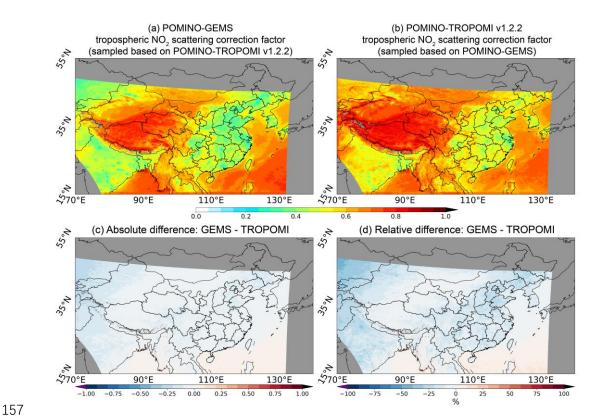


Figure S12. Spatial distribution of (a) POMINO-GEMS and (b) POMINO-TROPOMI v1.2.2 tropospheric NO<sub>2</sub> scattering correction factors on a  $0.05^{\circ} \times 0.05^{\circ}$  grid in JJA 2021. (c) and (d) are absolute and relative differences of POMINO-GEMS tropospheric NO<sub>2</sub> scattering correction factors from those of POMINO-TROPOMI v1.2.2, respectively. Data are sampled from locations and times with valid NO<sub>2</sub> VCD data in both POMINO-GEMS and POMINO-TROPOMI v1.2.2. The regions in grey mean there are no valid NO<sub>2</sub> observations.

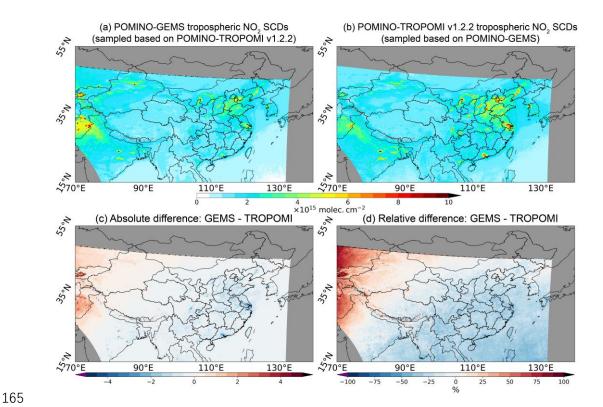


Figure S13. Spatial distribution of (a) POMINO-GEMS and (b) POMINO-TROPOMI v1.2.2 tropospheric NO<sub>2</sub> SCDs on a  $0.05^{\circ} \times 0.05^{\circ}$  grid in JJA 2021. (c) and (d) are absolute and relative differences of POMINO-GEMS tropospheric NO<sub>2</sub> SCDs from those of POMINO-TROPOMI v1.2.2, respectively. Data are sampled from locations and times with valid NO<sub>2</sub> VCD data in both POMINO-GEMS and POMINO-TROPOMI v1.2.2. The regions in grey mean there are no valid NO<sub>2</sub> observations.

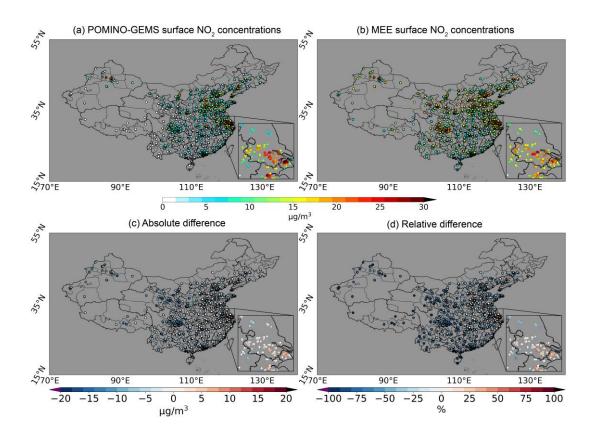


Figure S14. Evaluation of POMINO-GEMS derived surface NO<sub>2</sub> concentrations. Mean surface NO<sub>2</sub> concentrations (a) derived from POMINO-GEMS VCDs and (b) taken from MEE measurements in JJA 2021. Panels (c) and (d) are the absolute and relative differences of POMINO-GEMS relative to MEE. The sub-figures show a zoomed-in map around the Yangtze River Delta (YRD) region (118-122°E, 30-34°N).

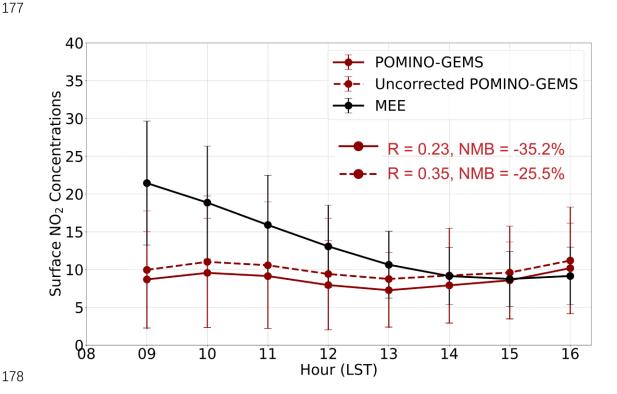


Figure S15. Diurnal variation of hourly surface NO<sub>2</sub> concentrations (μg m<sup>-3</sup>) of MEE (back line), POMINO-GEMS with TROPOMI correction (red solid line) and without TROPOMI correction (red dashed line) using daily GEOS-Chem column-to-surface ratios in JJA 2021. The error bars denote the standard deviation of MEE and POMINO-GEMS derived surface NO<sub>2</sub> concentrations at each hour in JJA 2021, respectively. Values for diurnal correlation and mean NMB of POMINO-GEMS relative to MEE data are shown.



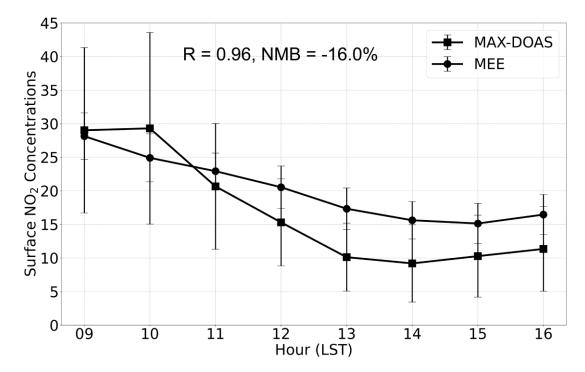


Figure S16. Diurnal variation of hourly surface NO<sub>2</sub> concentrations (μg m<sup>-3</sup>) for MEE (circle marks) and MAX-DOAS (square marks) in JJA 2021. The error bars denote the standard deviation of MEE and MAX-DOAS derived surface NO<sub>2</sub> concentrations at each hour in JJA 2021, respectively. Values for diurnal correlation and mean NMB of MAX-DOAS derived surface NO<sub>2</sub> concentrations relative to MEE data are shown.

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