



Supplement of

Towards an integrated inventory of anthropogenic emissions for China

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S1 Sectoral emission changes with implementation of mitigation

In this section, we discuss the implementation of mitigation in China, the differences in emissions between emission inventories, and the representation of emission inventories in relation to strategies.

According to the literature review, during the 11th nationwide five-year emission control plan, which started in 2010, China implemented stringent policies targeting coal combustion, fossil fuel combustion and NO_x emitters in various sectors. As shown in Figure S1a, these measures, including the introduction of ultra-low emission technologies and new vehicle standards, successfully reduced pollutants such as SO₂ and CO around 2010, contributing to cleaner air and addressing multiple sources of pollution. During the period of ‘Air Pollution Prevention and Control Action Plan’ (Plan, 2013), the government targeted PM_{2.5} and PM₁₀ reductions. Measures focused on energy conversion (coal-to-gas and coal-to-electricity), phasing out old vehicles and improving fuel quality (12th Five-Year Plan, 2011). The next phase of the ‘Three-Year Action Plan to Combat Air Pollution’ focuses on reducing PM_{2.5} and controlling VOC emissions by tackling pollution from diesel-powered trucks and treating industrial furnaces and ovens (Blue sky plan, 2018). The FAP first mentioned the co-benefits of air pollution control and climate change mitigation, leading to a significant reduction in carbon emissions. The national 14th Five-Year Plan (2021-2025) aims to peak CO₂ emissions before 2030 and achieve carbon neutrality before 2060, which would help reduce projected global warming by about 0.2 to 0.3 degrees Celsius (14th Five-Year Plan, 2020). Concrete measures include boosting the new energy vehicle industry and adapting and transforming energy and technology systems. The challenge for emission inventories is to depict or describe the rapid changes in emissions, including peak years, trends and amounts from sources. Pollutants such as CO and NO_x are gradually falling below the WHO standard due to measurement (Figure S1b), but ozone is still above the standard and shows a rising trend.

As a result of the above measures, shifts in individual sectoral emissions were rapid and were not captured by some global emission inventories. This was a major source of uncertainty in the emission inventories. Bottom-up emission inventory compilers, such as EDGAR, adopted emission factors and activity data statistics from IPCC in 2006 to ensure temporal consistency over time and comparability between countries. However, national emission inventories use a methodology that aggregates removal efficiency parameters based on specific pollution control technologies (Li et al., 2017; Zheng et al., 2018; Hoesly et al., 2018). In addition, the underlying data from the National Bureau of Statistics, including activity rates and penetration of different technologies, differ across sectors and provinces (Zhang et al., 2007, 2009). Therefore, these differences in the construction of emission inventories lead to different emission amounts in national and global emission inventories. In order to limit the uncertainties, many global emission inventories have included key sectoral emissions from regional and national emission inventories, as discussed in previous sections. However, global emission inventories, such as CEDS and HTAPv3, use total emissions from national emission inventories for specific species and sectors, and allocate emissions on the grid using proxy data. This process can also lead to inconsistencies in the spatial distribution between emission inventories, and the proxy data sources used by emission inventories are discussed in a later section.

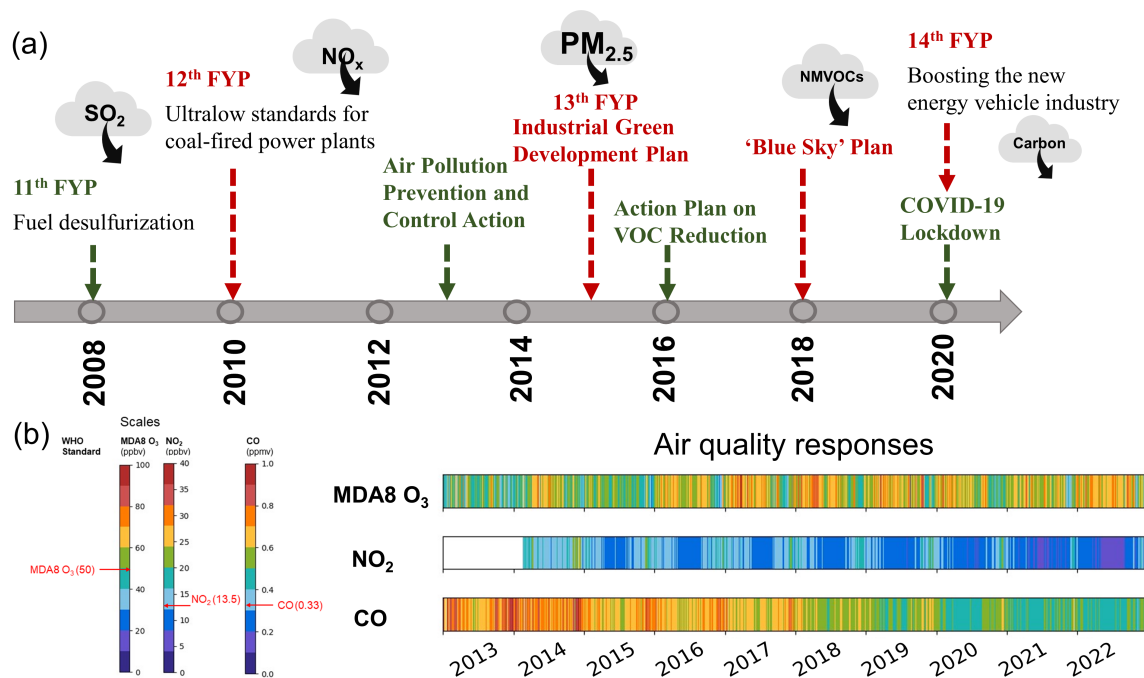


Figure S1. Implementation of air pollution and carbon emission strategies over the years from 2008 to 2020 (a). Observed concentrations for MDA8 ozone (ppbv), NO₂ (ppbv) and CO (ppmv) in daily resolution over April to October (warm seasons) from 2013 to 2022. The values with red color on the color bar indicate WHO guideline values (b).

S2 Differences in activity data and emission factors Used by emission inventories

In bottom-up emission inventories, emissions are calculated by multiplying the emission factor by the driver data (activity data) for a total emission for a given region and sector (Hoesly et al., 2018). Emission inventory compilers treat all emission sectors as two categories: fuel combustion sectors and non-combustion sectors, due to the different use of emission factors and activity data (Zheng et al., 2018). Fuel combustion sectors include all sub-sectors under 1A, such as energy transformation processes, including coal and coke production, charcoal production, and petroleum refining, etc., as listed in Table S1. It includes nitrogen oxides (NO_x), sulfur dioxide (SO₂), carbon monoxide (CO), black carbon (BC), organic carbon (OC), etc. The emission inventories are derived with sectors, species, time and regions, and their unit is g g⁻¹. Global emission inventories, such as Emissions Database for Global Atmospheric Research (EDGAR), by default estimate emissions via emission factors from the database of Greenhouse Gas – Air Pollution Interactions and Synergies (GAINS, <https://iiasa.ac.at/models-tools-data/gains>, last accessed: June, 2024) model, the United States National Emissions Inventory (NEI, <https://www.epa.gov/air-emissions-inventories/national-emissions-inventory-nei>, last accessed: June, 2024) energy use, and so on. Activity sectors are described as energy consumption, from the International Energy Agency (IEA) database. And emissions from non-combustion sectors, including waste, agricultural activities, are calculated by multiplying emission factors by population for a given activity. The national Multi-resolution Emission Inventory for China (MEIC) emission inventory followed the methodology of the global inventories, making adjustments in the calculation and updating the underlying data (Zheng et al., 2018). Specifically, a parameter (η) is added to the emissions calculation to constrain emissions taking into

50 account abatement. η represents technology penetration and abatement efficiencies. Therefore, the activity rates of energy consumption are derived from China's energy statistics. Community Emissions Data System (CEDS) and Hemispheric Transport of Air Pollution (HTAP) emission inventory currently use the 'MOSAIC' approach to scale national MEIC emission inventory to their global emission inventory for China. Specifically, CEDS adopted the reported emission amounts from MEIC and calculated new emission factors via emissions divided by activity data. CEDS kept the emission factors for China with temporal
55 variation and different among provinces. HTAP emission inventory did not update the emission factors, but scaled the total emission amount for China by sector mapping.

Table S1: Comparisons of underlying data used for emission factor, activity data in global and national emission inventories.

Sectors	emission inventories	Parameters	Underlying data sources
Fuel combustion	EF	Global	Nemission inventory from EPA and EEA ¹
	AD	National	Nemission inventory and Local measurement ²
		Global	IEA energy statistics ³
Non-combustion	AD	National	National Bureau of Statistics ⁴
		national	Selective (non-)catalytic reduction system ⁵
	C, η	Global	EDGAR, ECLIPSE ⁶
Non-combustion	EF	National	Nemission inventory and Local measurement
	AD	Global	Population data from FAO ⁷
		National	Chinese statistical yearbooks
	C, η	National	Selective (non-)catalytic reduction system

¹National Emission Inventory (NEI, <https://www.epa.gov/air-emissions-inventories/national-emissions-inventory-nei>, last accessed: June, 2024), European Environment Agency (EEA), and Environmental Protection Agency (EPA)

²data collected from priory studies(Qian, 2010; Zhang et al., 2016; Cheng et al., 2010).

³International Energy Agency (IEA, <https://www.iea.org/data-and-statistics>, last accessed: June, 2024)

⁴<https://www.stats.gov.cn/sj/ndsj/2015/indexch.htm>, last accessed: June, 2024

⁵(Guo et al., 2014)

⁶Project for Evaluating the Climate and Air Quality Impact of Short-Lived Pollutants

⁷Food and agriculture organization <https://www.fao.org/faostat/en/>, last accessed: June, 2024

S3 Differences in Spatial Proxies Used by emission inventories

Emission data is firstly provided as country-specific and sector-specific emissions. Then, emission compilers allocate total emissions to grid cells using sectoral proxy datasets (Feng et al., 2020a). These proxy data represent the spatial distribution of emissions, which is associated with the geographic coordinates of human activities. However, different geographic information is utilized by inventory compilers, such as road network maps in the transportation sector, power plant locations in the energy sector, etc., as listed in Table S2. The proxy datasets provided by the EDGAR dataset are widely used by global emission inventories, and global gridded emissions have spatial correlation structures, while errors in emissions may be correlated to systematic errors. This type of error or uncertainty stems from inaccurate spatial proxy data that do not accurately reflect the actual spatial distribution of emissions. One example is sulfur dioxide (SO₂) emissions. These tend to be overestimated in urban areas and underestimated in rural areas. The national inventory (MEIC) uses provincial Gross Domestic Product (GDP) data to constrain and map emissions from the country to provinces before gridding. This approach potentially improves the accuracy of estimated urban and rural emissions. MEIC also utilizes more localized geographic datasets to generate proxy data, aiming to capture a more accurate spatial distribution. Notably, spatial proxies remain empirical and may have introduced significant uncertainties into the spatial distributions of emissions.

Table S2. Comparisons of proxy data sources for common sectors used in emission inventories.

Sectors	emission inventories	Geographic Data Source
Energy	National emission inventory	China coal-fired Power plant Emissions Database
	Global emission inventories	Carbon Monitoring for Action
Industry, Residential	National emission inventory	National Bureau of Statistics for population and GDP
	Global emission inventories	EDGAR-HYDE
Transport	National emission inventory	China Digital Road-network Map
	Global emission inventories	EDGAR-HYDE
Agriculture	National emission inventory	National Bureau of Statistics for rural population
	Global emission inventories	Digital Chart of the World (DCW)

S4 Comparisons of emissions between emission inventories' versions

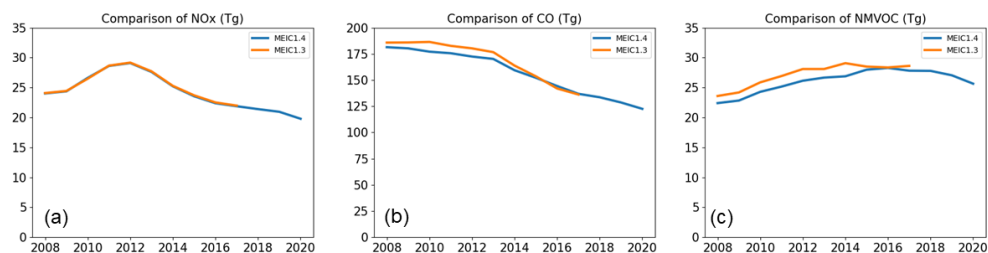


Figure S2. Interannual variations of total emissions (NO_x, CO and NMVOC) from version 1.3 and 1.4 of MEIC inventories, unit: Tg.

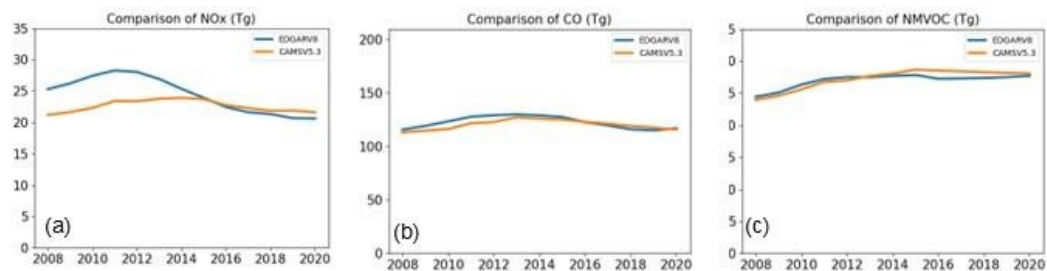


Figure S3. Interannual variations of total emissions (NO_x, CO and NMVOC) from CAMsv5 and EDGARv6, unit: Tg.

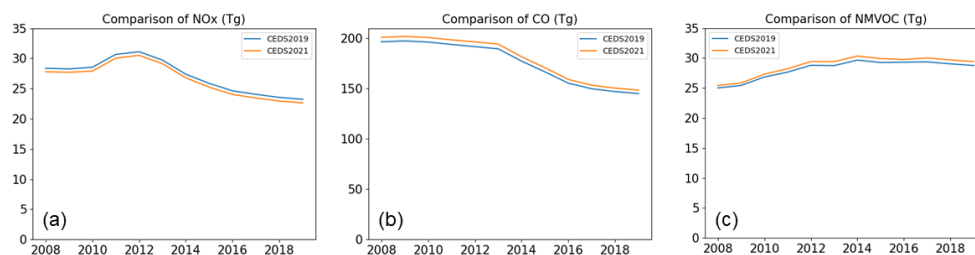


Figure S4. Interannual variations of total emissions (NO_x, CO and NMVOC) from version 2019 and 2021 of CEDS, unit: Tg.

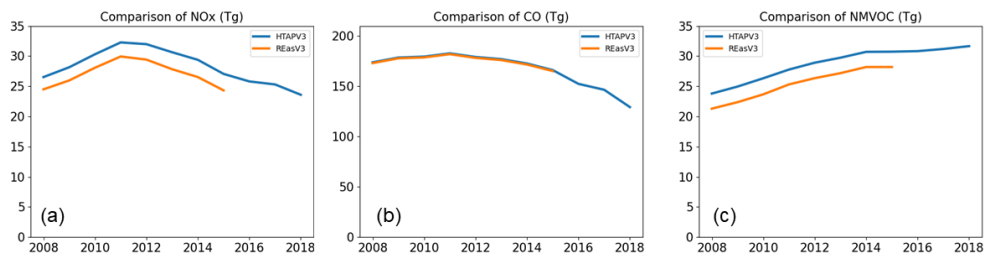


Figure S5. Interannual variations of total emissions (NO_x , CO and NMVOC) between HTAPv3 and REasv3.2.1, unit: Tg.

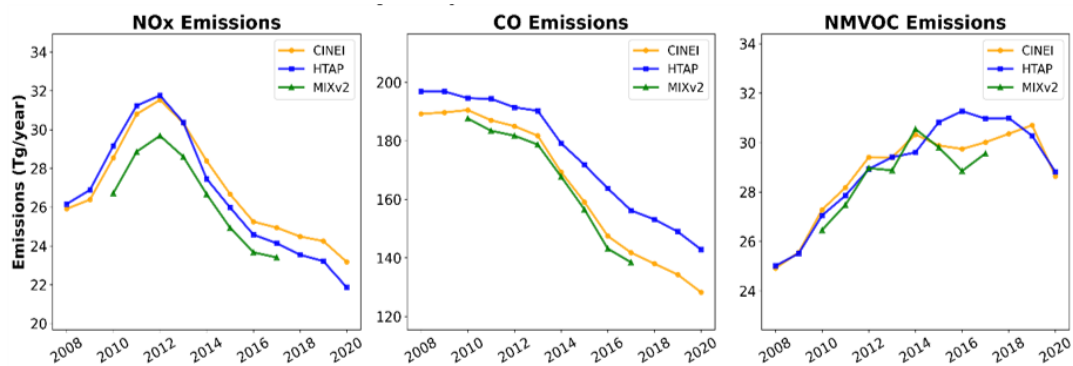


Figure S6. Interannual variability of total NO_x (NO_2), CO and NMVOC emissions in China from the CINEI in orange (2008 to 2020) and MIXv2 in green (2010 to 2017), and HTAPv3.1 in blue (2008 to 2020).

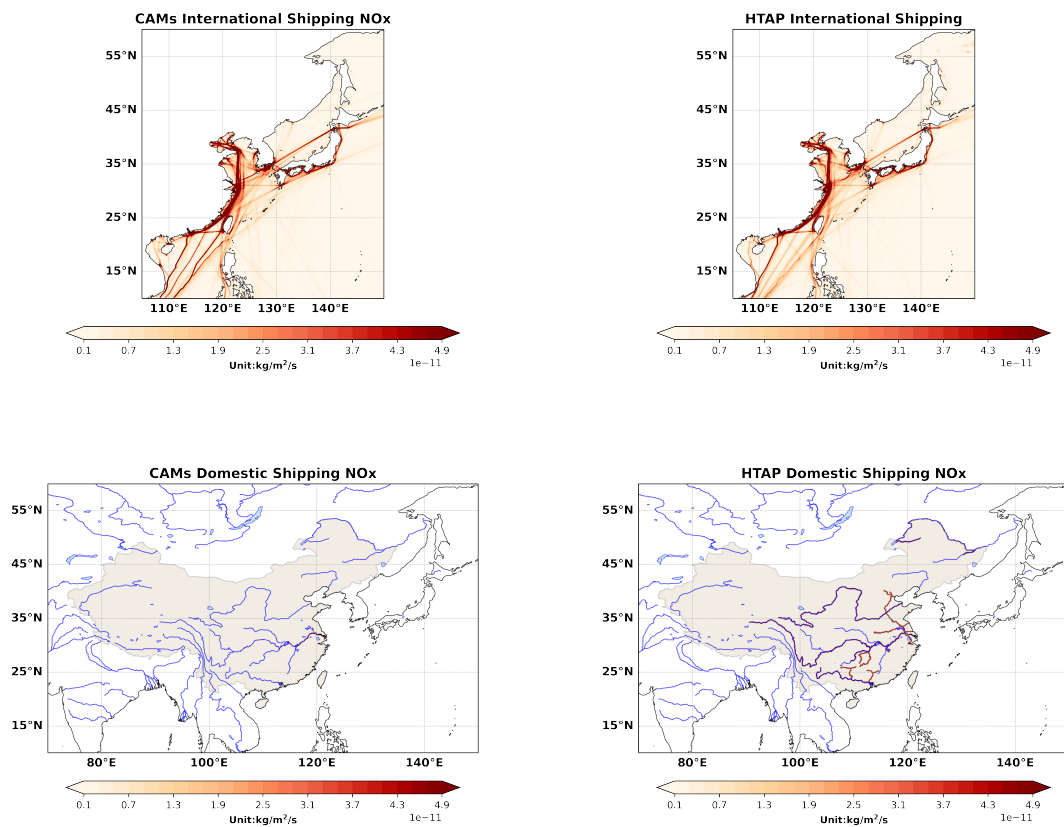


Figure S7. Spatial distribution of international shipping and inland shipping of CAMs and HTAP.

S5 Comparison of HTAPv3.1, MIXv2.1 and CINEI

When comparing the HTAPv3.1, MIXv2 and CINEI inventories, the main advantages of CINEI are:

1. Broader emission sectors in CINEI, including aviation and domestic ships, are missing from the MIXv2 inventory (see Table 2 in Li et al. (2024b)). MIXv2 presents only seven broad sectors in gridded format and lacks the detailed 22 subsectors in time series, which are available in MEIC v1.4. As shown in Fig. S10-S12, MIXv2 is limited in its ability to analyse subsector emission trends over time and complicates direct sector mapping with global inventories. For example, Table 2 in Li et al. (2024b) provides a one-way mapping between MIXv2 and the IPCC code. Figure S8 provides a two-way mapping, including one between the CINEI and the IPCC code and one between the existing inventories and the IPCC code. Therefore, the missing sub-sectors like complicating direct sector mapping with global inventories. Enteric Fermentation (3A) missing by MIXv2 and Wastewater treatment and discharge (4D) missed by MIXv2 and HTAP can be screened.
2. Updated NMVOC speciation profiles in CINEI that are fully compatible with the MOZART chemistry mechanism, which is widely adopted in air quality studies and regional chemistry and transport models (CTMs), such as the Weather Research and Forecasting (WRF) model coupled with Chemistry (WRF-Chem), the Community Earth System Model (CESM) and the Multi-Scale Infrastructure for Chemistry and Aerosols (MUSICA) (Dai et al., 2023; Mariscal et al., 2025; Danabasoglu et al., 2020; Dai et al., 2024). The MIXv2 inventory provides speciations such as CB05 and SPARC that are suitable for certain regional and chemistry models; while HTAPv3.1 currently lacks local profile updates for NMVOC species and the speciated NMVOC emissions in gridded format have not yet been completed (Guizzardi et al., 2025).
3. Facilitation of widely used chemistry mechanisms for global climate models. CINEI's integration with the global CEDS inventory further enhances its applicability for climate change studies, including use within the Coupled Model Inter-comparison Project (CMIP) framework (Feng et al., 2020b). CINEI is compatible with the MOZART chemistry mechanism that is widely adopted in air quality studies and regional chemistry and transport models; This broad compatibility positions CINEI as a flexible and valuable resource for a wide range of modeling applications.

Figure S6 shows a comparison of the interannual variation in NO_x , CO, and NMVOC emissions among CINEI, MIXv2, and HTAPv3.1. For the overlapping period (2010–2017), the inventories show minor discrepancies. On average, annual emissions in HTAPv3.1 are 2.1% higher than CINEI (ranging from -0.8% to +5.8% across different species), while MIXv2 emissions are consistently 3.2% lower (ranging from -1.6% to -6.1%). These differences mainly result from variations in sectoral aggregation methodologies. For instance, NO_x emissions in CINEI and HTAPv3.1 are higher than in MIXv2, with annual differences of 1.5 Tg (5%), mainly due to the omission of aviation (1.1 Tg) and agricultural soil emissions (0.3 Tg) in MIXv2. Annual CO emissions from agricultural waste burning in HTAPv3.1 are 5 Tg higher than in CINEI and MIXv2. Although both CINEI and MIXv2 provide speciated NMVOC emissions compatible with chemistry mechanisms, HTAP currently lacks local profile updates for NMVOC species.

105 S6 uncertainties in the projection of CAM emissions from 2018 onwards

For this study, CAMs emissions for the main sectors (industry, power, residential and transportation) from 2018 to 2020 are extrapolated using linear slope_{spec,i} derived from CEDS for the period 2015 to 2019, with 2018 as the base year. The emissions for a given species (spec) and sector (i) in years 2019–2020 are calculated as:

$$E_{\text{spec,year},i} = E_{\text{spec,2018},i} + \text{slope}_{\text{spec},i} \times (\text{year} - 2018) \quad (\text{S1})$$

- 110 Here, slope_{CEDS, spec,i} is the slope of linear regression of annual total CEDS emissions for sector i and specific species (spec) from 2015 to 2019 and slope_{CINEI, spec,i} is the slope of linear regression of annual total CINEI emissions. The uncertainty of the linear slope is calculated as the absolute difference between linear slopes of CINEI and CEDS from 2015 to 2019 with respect to their averages. The calculation is expressed as:

$$\sigma_{\text{slope}} = \frac{|\text{slope}_{\text{CEDS, spec},i} - \text{slope}_{\text{CINEI, spec},i}| \times 2}{\text{slope}_{\text{CEDS, spec},i} + \text{slope}_{\text{CINEI, spec},i}} \times 100 \quad (\text{S2})$$

- 115 The uncertainty of the bias is calculated as the absolute difference of CAMs and CINEI emissions with respect to their average in the base year.

$$\sigma_{\text{bias2018}} = \frac{|E_{\text{CAMs,spec,2018},i} - E_{\text{CINEI,spec,2018},i}| \times 2}{E_{\text{CAMs,spec,2018},i} + E_{\text{CINEI,spec,2018},i}} \times 100 \quad (\text{S3})$$

- The uncertainty of the model (σ_{model}) originates from differences in approaches to calculate emissions, including top-down estimation (satellite estimation and inverse modeling) and bottom-up estimation (Miyazaki et al., 2017; Li et al., 2024b; Liu et al., 2016a). This component is independent of the uncertainties of linear slope and base-year emission in bottom-up emission inventories. Adopted from Li et al. (2024a), the standard deviation of all estimates on emission trends can be represented by 46% for NO_x, 39% for CO, and 26% for NMVOC. The propagation of uncertainty for three independent uncertainties is expressed as follows:

$$\sigma_{\text{total,spec},i} = \sqrt{\sigma_{\text{slope,spec},i}^2 + \sigma_{\text{model,spec},i}^2 + \sigma_{\text{bias,spec},i}^2} \quad (\text{S4})$$

Table S3. Comprehensive uncertainty table for CAMs Emissions Extrapolation Method: CO, NOx, and NMVOC by Sector

Species	Sector	Slopes (Tg/year)			Emission in base year (2018)			σ_{model}	σ_{total}
		CEDS	CINEI	σ_{slope} (%)	CAMs (Tg)	CINEI (Tg)	σ_{bias} (%)	(%)	(%)
CO	Transportation	-1.6021	-1.5969	0.3	14.83	23.67	45.9	39.0	60.2
	Residential	-2.1838	-2.2927	4.9	27.34	55.81	68.5	39.0	78.8
	Power	0.0692	0.1850	91.1	12.80	5.01	87.5	39.0	95.8
	Industry	-1.3966	-2.2350	46.2	75.49	47.67	45.2	39.0	59.7
NOx (NO2)*	Transportation	-0.0160	-0.1717	165.8	5.2	7.5	35.0	46.0	57.8
	Residential	-0.0229	-0.0267	15.5	1.0	0.8	17.3	46.0	49.2
	Power	-0.1439	-0.2977	69.7	6.3	4.0	44.1	46.0	63.7
	Industry	-0.0956	-0.1608	50.9	8.5	9.1	7.2	46.0	46.6
NMVOC†	Transportation	-0.2747	-0.2145	24.6	3.89	4.63	17.4	26.0	31.3
	Residential	-0.2069	-0.0941	74.9	3.05	4.67	42.1	26.0	49.5
	Power	0.1204	-0.0024	208.2	0.49	0.08	146.0	26.0	148.3
	Industry‡	-0.0046	0.5275	203.5	20.19	19.49	3.5	26.0	26.2

Notes:

- * CAMs NOx (represented by NO) emissions scaled by factor 1.5
- ‡ Industry sector for NMVOC includes solvents (ind + slv)
- Slopes calculated from linear regression (2015-2019)
- Base year emissions in appropriate units for each species
- Uncertainties calculated using equations (2)-(4) from methodology
- Model uncertainties: CO (39%), NOx (46%), NMVOC (26%) from Li et al. (2024b).

125 Table S3 presents the uncertainties of CAMs emissions in main sectors. The total uncertainties of the CAMs extrapolation
method range from 30% to 60%. The largest outlier uncertainties are in the power sector, with 96% for CO emissions and 148%
for NMVOC emissions. These abnormal uncertainties are likely attributed to systemic uncertainty due to the sector definition
of CAMs in the power and industry sectors. The uncertainty of the model’s estimation (bottom-up and top-down approaches)
adopted from literature is smaller than the extrapolated method used in the CAMs data (20-50%). Therefore, a combined
130 method using activity data, in-situ measurements, satellite data, and CTM modeling is recommended to reduce uncertainty for
our future work.

CINEI	IPCC sector	MEIC	CEDS ¹	CAMs ²	HTAP ³	EDGAR ⁴
Power from MEIC	1A1a_Public electricity and heat production	Power	Power	Power	Power	Power
Industry from MEIC	1A1bc_Other Energy Industries	Industry	Industry	Industry	Industry	Industry
	1B1_Solid Fuels					
	1B2_Fugitive emissions from oil and gas					
	1B3_Other Emission from Energy Production					
	5B_Fossil fuel fires					
	1A2_Manufacturing Industries and Construction					
	2A1_Cement production					
	2A2_Lime production					
	2A4_other process use of Carbonates					
	2A7_Production of other minerals					
	2B_Production of chemicals					
	2C_Production of metals					
	2D_Production of (no-energy) solvent use					
	2D_Production of (no-energy) pulp/paper/food/dr					
Residential from MEIC	1A4_Residential and other sectors		Residential	Residential	Residential	
	1A5_Other Energy Industries					
Aviation from HTAP	1A3a_Civil aviation			Aviation	Aviation	
Transport from MEIC	1A3b_Road transportation resuspension	Transport	Transport	Transport	Transport	Transport
	1A3c_Rail transportation					
	1A3e_Other transportation					
Domestic Ships from CAMs	1A3d_Inland (Domestic) navigation			Ships	Ships	Ships
International Ships from HTAP	1A3d_Water-borne (International) navigation		Ships			
Agriculture from HTAP	3A_Enteric Fermentation	Agriculture For NH ₃	Agriculture	Agriculture	Agriculture	
	3B_Manure management					Agriculture
	3C_Rice Cultivation	Agriculture For NH ₃				
	3D_Agriculture soils					
	3F_Field burning of agriculture residues					
Waste from CEDS	4A_Solid Waste Disposal		Waste	Waste	Waste	Waste
	4B_Biological Treatment of Solid Waste					
	4C_Incineration and Open Burning of Waste				Waste	
	4D_Wastewater Treatment and discharge					
	4E_other				Waste	

Figure S8. Harmonized sectors from all inventories aligned with IPCC2006 sectors. For good comparison, we have standardized the definition of gridded sectors from all inventories as 8 harmonized sectors. In CEDS we combine original solvent and residential sector as harmonized residential sector. In CAMs, we combine the original solvent and residential sectors as the harmonized residential sector. We also combine original fugitive and industrial sectors as a harmonized industrial sector. We combine non-road and road transport as transport. In HTAP, we combine 'transportation on the road', 'Brake and tyre wear' and 'other transportation' as harmonized transport sector. We also combine the 'Agricultural livestock', 'agricultural crops', and 'Agricultural waste burning' as harmonized agriculture sectors. In EDGAR, we combine the original solvent sector and the building sector as the harmonized housing sector.

Table S4: Mapping table of modeling MOZART species between MEIC emission inventory and global emission inventory (CEDS), used for harmonized emission inventories.

WRF_Chem MOZART species	VOC groups	Species name	MEIC species	global emission inventory species
C ₂ H ₆	alkanes	ethane	ETHA	VOC02-ethane
C ₃ H ₈	alkanes	propane	ALK2	VOC03-propane
BIGALK	alkanes	butanes	ALK3	VOC04-butaness
BIGALK	alkanes	pentanes	ALK4	VOC05-pentanes
BIGALK	alkanes	hexanes	AKL5	VOC06-hexanes-pl
C ₂ H ₄	alkenes	ethene	ETH	VOC07-ethene
C ₃ H ₆	alkenes	propene	HC3	VOC08-propene
BIGENE	alkenes	butenes	IOLE	VOC22-other-alka
C ₂ H ₂	alkynes	acetylene	CO*Ratio	CO*Ratio
ISOP	alkynes	Isoprene	ISOP	VOC22-other-alka*Ratio
C ₁₀ H ₁₆	alkynes	3-methylbutanal	TERP	VOC22-other-alka*Ratio
BENZENE	aromatics	benzene	TOL*Ratio	VOC14-toluene*Ratio
TOLUENE	aromatics	toluene	TOL*Ratio	VOC14-toluene
XYLENE	aromatics	xylene	XYL	VOC15-xylene
CH ₂ O	OVOCs	formaldehyde	FORM	VOC23-ketones*Ratio
CH ₃ CHO	OVOCs	acetaldehyde	ACET	VOC23-ketones*Ratio
C ₂ H ₅ OH	OVOCs	ethanol	ETOH	VOC01-alcohols*Ratio
CH ₃ OH	OVOCs	methanol	MEOH	VOC01-alcohols*Ratio
MGLY	OVOCs	methyl glyoxal	MGLY	n.a.
MEK	OVOCs	methyl ethyl ketone	MEK	n.a.
CH ₃ COCH ₃	OVOCs	acetone	ACET	VOC23-ketones*Ratio
MVK	OVOCs	methyl ethyl ketone	MVK	VOC23-ketones*Ratio
GLY	OVOC	glyoxal	GLY	n.a.

The ratios are adopted from Carter (2015).

n.a. indicates that the species is not present in the inventories.

Table S5: Mapping table of main categories of sources in source profiles to CINEI

Categories in source profile	source profile	CINEI
Sationary combustion	Sha et al. (2021)	Power
Solvent use/Industrial process	Mo et al. (2016)	Industry
Fossil fuel burning	Mo et al. (2016)	Residential
Transportation	Mo et al. (2016)	Transportation
Biomass burning	Mo et al. (2016)	Agriculture
Waste incineration	Sha et al. (2021)	Waste
Transportation	Mo et al. (2016)	Aviation
Transportation	Mo et al. (2016)	Shipping

Table S6: Maximum incremental reactivity (MIR) of individual NMVOC species (Unitless).

SPECIE NAME	Maximum incremental reactivity	mapping to modeling species
Ethane	0,28	C ₂ H ₆
Propane	0,49	C ₃ H ₈
i-Butane	1,15	BIGALK
n-Butane	1,15	BIGALK
Cyclopentane	2,39	BIGALK
i-Pentane	1,45	BIGALK
n-Pentane	1,31	BIGALK
Methylcyclopentane	2,91	BIGALK
Cyclohexane	1,25	BIGALK
2,2-Dimethylbutane	1,17	BIGALK
2,3-Dimethylbutane	0,97	BIGALK
2-Methylpentane	1,50	BIGALK
3-Methylpentane	1,80	BIGALK
n-Hexane	1,24	BIGALK
Methylcyclohexane	1,70	BIGALK
2,3-DimethylPentane	1,34	BIGALK
2,4-Dimethylpentane	1,55	BIGALK
2-Methylhexane	1,19	BIGALK
3-Methylhexane	1,61	BIGALK
n-Heptane	1,07	BIGALK
2,2,4-Trimethylpentane	1,26	BIGALK
2,3,4-Trimethylpentane	1,03	BIGALK
2-Methylheptane	1,07	BIGALK
3-Methylheptane	1,24	BIGALK
n-Octane	0,90	BIGALK
n-Nonane	0,78	BIGALK
n-Decane	0,68	BIGALK
n-Un.a.ecane	0,61	BIGALK
Ethene	9,00	C ₂ H ₄
Propene	11,66	C ₃ H ₆
1,3-butadiene	12,61	BIGENE
1-Butene	9,73	BIGENE
cis-2-Butene	14,24	BIGENE
trans-2-Butene	15,16	BIGENE
Isoprene	10,61	ISOP
1-Pentene	7,21	BIGENE

Table S6 continued from previous page

SPECIE NAME	Maximum incremental reactivity	mapping to modeling species
cis-2-Pentene	10,38	BIGENE
trans-2-Pentene	10,56	BIGENE
1-Hexene	5,49	BIGENE
Ethyne	0,95	C ₂ H ₂
Benzene	0,72	BENZENE
Toluene	4,00	TOLUENE
m/p-Xylene	7,80	XYLENES
Ethylbenzene	3,04	XYLENES
o-Xylene	7,64	XYLENES
Styrene	1,73	XYLENES
1,2,3-Trimethylbenzene	11,97	XYLENES
1,2,4-Trimethylbenzene	8,87	XYLENES
1,3,5-Trimethylbenzene	11,76	XYLENES
i-Propylbenzene	2,52	XYLENES
m-Ethyltoluene	5,49	TOLUENE
n-Propylbenzene	4,44	XYLENES
o-Ethyltoluene	5,49	TOLUENE
p-Ethyltoluene	5,49	TOLUENE
m-Diethylbenzene	7,10	XYLENES
p-Diethylbenzene	4,43	XYLENES
tetrachloromethane	0,00	NROG
Chloroform	0,04	NROG
Dichloromethane	0,00	NROG
Chloromethane	0,04	NROG
Tetrachloroethylene	0,04	NROG
Vinyl chloride	0,04	NROG
Formaldehyde	9,46	CH ₂ O
Acetaldehyde	4.1	CH ₃ CHO
acrolein	7,54	GLY
Methanol	0,38	CH ₃ OH
Ethanol	0,66	C ₂ H ₅ OH
Propionaldehyde/Propanal	7,54	GLY
Butyraldehyde/n-Butanal	7,54	GLY
Valeraldehyde/n-Pentanal	7,54	GLY
Isovaleraldehyde	7,54	GLY
Benzaldehyde	7,54	GLY
Hexanaldehyde/n-Hexanal	7,54	GLY

Table S6 continued from previous page

SPECIE NAME	Maximum incremental reactivity	mapping to modeling species
Acetone	0,36	MEK
Methyl ethyl ketone/Butanone	3,88	MVK
isopropanol	0,61	NROG
ethyl acetate	0,07	CH ₃ COOH

The MIR values are adopted from Carter (2015).

S7 Setups of the WRF-Chem model and evaluation of the model

Table S7. Setups of the WRF-Chem model.

Model Parameters	Descriptions
Simulation Periods	January and July 2017
Spin-up Periods	December 26th to December 30th, 2016 June 25th to June 30th, 2017
Horizontal Resolution	36 km (outer domain), 12 km (inner domain)
Vertical Resolution	33 eta levels up to 50 hPa
Meteorological Initial/Boundary Conditions	ERA5, 3-hourly
Chemical Initial/Boundary Conditions	CAM-Chem outputs, 6-hourly
Microphysics	Purdue-Lin (Gharaylou et al., 2009)
Cumulus Parameterization	New Tiedtke (Janjić, 1994)
Shortwave Radiation	RRTMG (Iacono et al., 2008)
Longwave Radiation	New Goddard (Chou and Suárez, 1999)
Land-surface	Noah Land Surface Model (Liu et al., 2016b)
Planetary Boundary Layer	Mellor-Yamada-Janjie (Nakanishi and Niino, 2009)
Gas Phase Chemical Mechanism	MOZART
Aerosol Scheme	MOSAIC
Photolysis Scheme	Madronich F-TUV

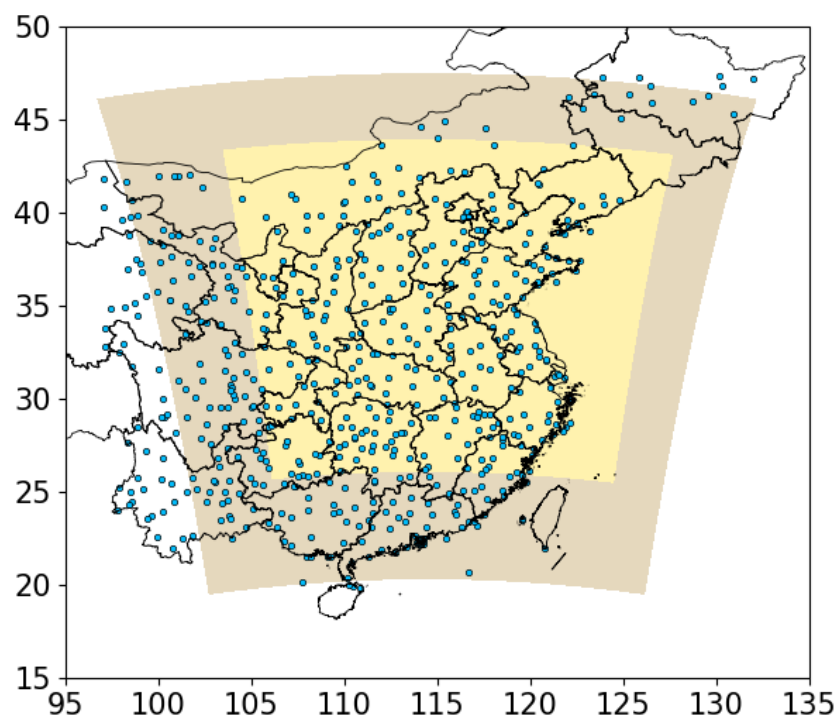


Figure S9. Spatial distribution of meteorological sites.

135 Several statistical metrics (Table S8) were employed to quantify the performance of each inventory: $\bar{O}$ is the average of
 observations at all sites in the region of interest (Fig. 2 in the main text), and N is the number of all available sites. The
 subscript i represents every individual site. P_i is the pixel of model grid including site i. For the multiple sites in the same
 pixel, we calculated the average of sites to compare with corresponding modeling values M_{P_i} . $\bar{O}$ is the monthly average of all
 modeling pixels including observational sites (M_{P_i}), and it represents the modeling result of each case, and can be validated by
 140 $\bar{O}$.

Table S8. Statistical metrics used for model validation, their calculation formulas, ranges, and the information provided from their values.

Metrics	Calculation Formulas	Ranges	Information
NMB	$\frac{\sum_{i=1}^N (M_i - O_i)}{\sum_{i=1}^N O_i}$	[-1, +∞]	A good performance is expected when NMB is close to 0.
MNB	$\frac{1}{N} \sum_{i=1}^N \left(\frac{\bar{M}_i - \bar{O}_i}{\bar{O}_i} \right)$	[-1, +∞]	Indicates the direction of overestimation (positive values) and underestimation (negative values).
MFB	$\frac{\sum_{i=1}^N \bar{M}_i - \bar{O}_i}{\sum_{i=1}^N \bar{O}_i}$	[-2, 2]	Normal distribution of bias around zero.
MNAE	$\frac{1}{N} \sum_{i=1}^N \left(\frac{ \bar{M}_i - \bar{O}_i }{\bar{O}_i} \right)$	[0, +∞]	Use MNAE when comparing errors across different magnitudes, especially for high interquartile models.
MAE	$\frac{1}{N} \sum_{i=1}^N \bar{M}_i - \bar{O}_i $	[0, +∞]	Measures the absolute error in the original units of the data.
RMSE	$\sqrt{\frac{1}{N} \sum_{i=1}^N (\bar{M}_i - \bar{O}_i)^2}$	[0, +∞]	Evaluates the magnitude of error between predicted and observed values.
R	$\frac{\sum_{i=1}^N (M_i - \bar{M})(O_i - \bar{O})}{\sqrt{\sum_{i=1}^N (M_i - \bar{M})^2 \sum_{i=1}^N (O_i - \bar{O})^2}}$	[-1, 1]	Evaluates the linear relationship between the prediction and the observation.

O_i and M_i indicate the observational and modeled value of the data pair i, and N is the number of data pairs in the comparisons.

Table S9: Inter-annual emissions of NO_x (NO₂) from all emission inventories

Year	emission inventories	Transportation	Residential	Power	Industry	Agriculture	Ships	Aviation	Waste	Sum
2008	MEIC	7,60	0,97	7,77	7,70	0,00	n.a.	n.a.	n.a.	24,05
2009	MEIC	7,32	1,00	7,78	8,32	0,00	n.a.	n.a.	n.a.	24,41
2010	MEIC	7,66	1,03	8,63	9,12	0,00	n.a.	n.a.	n.a.	26,44
2011	MEIC	7,95	1,06	9,49	10,13	0,00	n.a.	n.a.	n.a.	28,63
2012	MEIC	8,48	1,08	9,07	10,50	0,00	n.a.	n.a.	n.a.	29,13
2013	MEIC	8,48	0,98	7,95	10,27	0,00	n.a.	n.a.	n.a.	27,67
2014	MEIC	8,13	0,95	6,18	9,98	0,00	n.a.	n.a.	n.a.	25,25
2015	MEIC	7,97	0,91	5,08	9,70	0,00	n.a.	n.a.	n.a.	23,66
2016	MEIC	7,70	0,88	4,64	9,26	0,00	n.a.	n.a.	n.a.	22,48
2017	MEIC	7,72	0,85	4,19	9,19	0,00	n.a.	n.a.	n.a.	21,95
2018	MEIC	7,38	0,818	3,99	9,20	0,00	n.a.	n.a.	n.a.	21,40
2019	MEIC	7,22	0,80	3,89	8,98	0,00	n.a.	n.a.	n.a.	20,90
2020	MEIC	6,79	0,79	3,73	8,43	0,00	n.a.	n.a.	n.a.	19,74
2008	CAMs	3,99	0,91	6,98	7,59	0,63	0,13	0,01	n.a.	20,24
2009	CAMs	3,89	0,92	6,70	8,08	0,66	0,13	0,01	n.a.	20,39
2010	CAMs	4,03	0,92	6,71	8,51	0,65	0,12	0,02	n.a.	20,97
2011	CAMs	4,42	0,95	6,83	9,06	0,65	0,12	0,02	n.a.	22,05
2012	CAMs	4,81	0,96	6,50	8,93	0,65	0,12	0,02	n.a.	22,00
2013	CAMs	5,02	0,98	6,67	8,86	0,68	0,12	0,02	n.a.	22,35
2014	CAMs	5,12	0,99	6,53	8,71	0,65	0,63	0,02	n.a.	22,65
2015	CAMs	5,38	1,01	6,13	8,71	0,68	0,67	0,02	n.a.	22,61
2016	CAMs	5,33	1,00	5,82	8,62	0,68	0,17	0,02	n.a.	21,65
2017	CAMs	5,29	0,99	5,51	8,54	0,67	0,13	0,02	n.a.	21,16
2018	CAMs	5,25	0,98	5,23	8,45	0,67	0,13	0,02	n.a.	20,73
2019	CAMs	5,20	0,97	4,96	8,37	0,66	0,56	0,02	n.a.	20,75
2020	CAMs	5,16	0,96	4,70	8,28	0,66	0,69	0,02	n.a.	20,48
2008	CEDS	7,11	1,68	11,16	6,81	0,66	0,01	n.a.	0,55	27,98
2009	CEDS	6,88	1,71	10,78	7,26	0,69	0,01	n.a.	0,59	27,92
2010	CEDS	7,00	1,78	10,13	7,93	0,68	0,02	n.a.	0,64	28,17
2011	CEDS	7,22	1,85	11,08	8,79	0,68	0,02	n.a.	0,69	30,32
2012	CEDS	7,65	1,92	10,74	9,05	0,69	0,01	n.a.	0,74	30,80
2013	CEDS	7,65	1,83	9,72	8,72	0,71	0,01	n.a.	0,79	29,43
2014	CEDS	7,40	1,76	7,82	8,58	0,69	0,01	n.a.	0,84	27,10
2015	CEDS	7,30	1,69	6,58	8,43	0,72	0,02	n.a.	0,83	25,57
2016	CEDS	7,05	1,61	6,25	7,87	0,72	0,02	n.a.	0,83	24,35
2017	CEDS	7,07	1,56	5,97	7,61	0,72	0,02	n.a.	0,83	23,78

Table S9 continued from previous page

Year	emission inventories	transportation	residential	power	industry	agriculture	ships	aviation	waste	sum
2018	CEDS	7,06	1,51	5,60	7,53	0,73	0,02	n.a.	0,83	23,28
2019	CEDS	7,11	1,49	5,29	7,52	0,73	0,02	n.a.	0,83	22,99
2008	HTAP	5,50	1,82	8,96	7,74	0,78	1,15	0,09	0,01	26,06
2009	HTAP	6,08	1,87	9,07	8,44	0,84	1,23	0,09	0,02	27,66
2010	HTAP	6,50	1,96	9,86	9,19	0,79	1,30	0,12	0,02	29,75
2011	HTAP	7,06	2,02	10,55	9,70	0,84	1,36	0,11	0,02	31,66
2012	HTAP	7,10	2,04	9,84	9,81	0,85	1,56	0,13	0,02	31,35
2013	HTAP	7,05	1,96	8,92	9,22	0,86	1,79	0,14	0,02	29,96
2014	HTAP	7,19	1,98	7,63	9,04	0,79	1,88	0,16	0,02	28,71
2015	HTAP	6,88	2,03	6,78	8,00	0,82	1,70	0,18	0,03	26,42
2016	HTAP	6,65	1,95	6,19	7,64	0,78	1,76	0,21	0,03	25,21
2017	HTAP	6,67	1,89	5,59	7,58	0,74	1,98	0,24	0,03	24,71
2018	HTAP	6,46	1,76	4,60	7,19	0,71	2,04	0,24	0,03	23,03

Table S10: Inter-annual emissions of CO from all emission inventories

Year	emission inventories	transportation	residential	power	industry	agriculture	ships	aviation	waste	sum
2008	MEIC	32.42	69.80	3.25	79.99	n.a.	n.a.	n.a.	n.a.	185.46
2009	MEIC	30.39	70.84	3.32	81.03	n.a.	n.a.	n.a.	n.a.	185.58
2010	MEIC	31.96	70.91	3.79	79.44	n.a.	n.a.	n.a.	n.a.	186.09
2011	MEIC	30.25	71.58	4.43	76.03	n.a.	n.a.	n.a.	n.a.	182.29
2012	MEIC	29.36	72.37	4.51	73.68	n.a.	n.a.	n.a.	n.a.	179.92
2013	MEIC	29.75	69.23	4.69	72.63	n.a.	n.a.	n.a.	n.a.	176.30
2014	MEIC	27.24	66.60	4.50	65.14	n.a.	n.a.	n.a.	n.a.	163.49
2015	MEIC	28.88	63.93	4.47	56.02	n.a.	n.a.	n.a.	n.a.	153.30
2016	MEIC	26.19	60.35	4.58	50.58	n.a.	n.a.	n.a.	n.a.	141.69
2017	MEIC	25.18	56.89	4.84	49.03	n.a.	n.a.	n.a.	n.a.	135.94
2018	MEIC	23.71	57.52	5.12	47.21	n.a.	n.a.	n.a.	n.a.	133.56
2019	MEIC	22.16	54.73	5.18	46.30	n.a.	n.a.	n.a.	n.a.	128.37
2020	MEIC	19.54	52.40	5.14	45.23	n.a.	n.a.	n.a.	n.a.	122.32
2008	CAMs	16.21	36.73	2.23	49.39	n.a.	0.01	0.00	n.a.	104.57
2009	CAMs	13.66	35.53	2.30	53.67	n.a.	0.01	0.01	n.a.	105.17
2010	CAMs	12.14	33.60	2.45	57.77	n.a.	0.01	0.01	n.a.	105.98
2011	CAMs	13.37	32.36	2.56	61.98	n.a.	0.01	0.01	n.a.	110.29
2012	CAMs	14.44	31.05	2.57	63.27	n.a.	0.01	0.01	n.a.	111.35
2013	CAMs	16.33	29.96	2.67	65.67	n.a.	0.01	0.01	n.a.	114.65
2014	CAMs	16.78	28.89	2.72	65.17	n.a.	0.07	0.01	n.a.	113.63
2015	CAMs	16.49	28.73	2.71	64.77	n.a.	0.07	0.01	n.a.	112.79
2016	CAMs	15.91	28.24	2.71	63.95	n.a.	0.02	0.01	n.a.	110.85
2017	CAMs	15.36	27.80	2.71	63.18	n.a.	0.02	0.01	n.a.	109.09
2018	CAMs	14.83	27.34	2.71	62.44	n.a.	0.02	0.01	n.a.	107.34
2019	CAMs	14.32	26.87	2.71	61.73	n.a.	0.08	0.01	n.a.	105.72
2020	CAMs	13.83	26.51	2.70	61.05	n.a.	0.09	0.01	n.a.	104.19
2008	CEDS	33.06	70.77	12.73	75.78	n.a.	0.00	n.a.	3.44	195.77
2009	CEDS	28.94	71.85	15.08	77.06	n.a.	0.00	n.a.	3.74	196.68
2010	CEDS	27.88	71.77	16.68	75.25	n.a.	0.00	n.a.	4.03	195.61
2011	CEDS	26.16	72.50	18.38	71.93	n.a.	0.00	n.a.	4.33	193.30
2012	CEDS	25.16	73.35	18.62	69.50	n.a.	0.00	n.a.	4.64	191.26
2013	CEDS	25.45	70.38	19.75	68.57	n.a.	0.00	n.a.	4.94	189.10
2014	CEDS	23.18	67.73	19.05	61.68	n.a.	0.00	n.a.	5.25	176.88
2015	CEDS	24.68	65.21	17.78	53.21	n.a.	0.00	n.a.	5.25	166.13
2016	CEDS	22.19	61.65	17.83	47.96	n.a.	0.00	n.a.	5.25	154.89
2017	CEDS	21.17	58.35	18.18	46.41	n.a.	0.00	n.a.	5.25	149.36

Table S10 continued from previous page

Year	emission inventories	transportation	residential	power	industry	agriculture	ships	aviation	waste	sum
2018	CEDS	19.50	57.24	18.08	46.55	n.a.	0.00	n.a.	5.25	146.61
2019	CEDS	18.02	56.50	18.00	46.93	n.a.	0.00	n.a.	5.25	144.71
2008	HTAP	28.55	58.41	1.53	84.55	0.45	0.28	0.03	0.01	173.80
2009	HTAP	28.97	59.23	1.39	88.17	0.44	0.30	0.03	0.01	178.55
2010	HTAP	28.76	59.75	1.65	88.51	0.44	0.31	0.04	0.01	179.47
2011	HTAP	30.12	56.96	2.03	92.78	0.45	0.33	0.04	0.01	182.72
2012	HTAP	30.91	54.14	1.82	91.34	0.46	0.38	0.04	0.01	179.10
2013	HTAP	30.71	50.79	1.70	92.82	0.47	0.43	0.05	0.01	176.98
2014	HTAP	31.02	49.46	1.57	89.56	0.47	0.45	0.05	0.01	172.61
2015	HTAP	30.68	49.34	1.59	83.53	0.48	0.41	0.06	0.01	166.09
2016	HTAP	27.82	46.58	1.63	75.39	0.47	0.42	0.07	0.01	152.39
2017	HTAP	26.75	43.91	1.72	73.10	0.48	0.48	0.08	0.01	146.52
2018	HTAP	23.32	39.08	1.86	63.97	0.48	0.49	0.08	0.01	129.29

Table S11: Inter-annual emissions of NMVOCs from all emission inventories

Year	emission inventories	transportation	residential	power	industry	agriculture	ships	aviation	waste	sum
2008	MEIC	6.57	5.58	0.06	11.34	0.00	n.a.	n.a.	n.a.	23.55
2009	MEIC	6.07	5.64	0.06	12.37	0.00	n.a.	n.a.	n.a.	24.14
2010	MEIC	6.06	5.69	0.07	14.00	0.00	n.a.	n.a.	n.a.	25.82
2011	MEIC	5.75	5.75	0.08	15.29	0.00	n.a.	n.a.	n.a.	26.87
2012	MEIC	5.63	5.80	0.08	16.53	0.00	n.a.	n.a.	n.a.	28.03
2013	MEIC	5.58	5.61	0.08	16.76	0.00	n.a.	n.a.	n.a.	28.03
2014	MEIC	5.12	5.43	0.08	18.38	0.00	n.a.	n.a.	n.a.	29.00
2015	MEIC	5.39	5.13	0.08	17.83	0.00	n.a.	n.a.	n.a.	28.42
2016	MEIC	4.96	4.85	0.08	18.38	0.00	n.a.	n.a.	n.a.	28.28
2017	MEIC	4.79	4.60	0.08	19.07	0.00	n.a.	n.a.	n.a.	28.53
2018	MEIC	4.36	4.80	0.06	18.57	0.00	n.a.	n.a.	n.a.	0.00
2019	MEIC	4.48	4.75	0.07	19.91	0.00	n.a.	n.a.	n.a.	29.21
2020	MEIC	4.23	4.55	0.06	18.31	0.00	n.a.	n.a.	n.a.	27.15
2008	CAMs	2.63	10.35	5.24	5.05	n.a.	0.00	n.a.	0.48	23.73
2009	CAMs	2.52	10.48	5.52	5.32	n.a.	0.00	n.a.	0.50	24.34
2010	CAMs	2.62	10.51	6.04	5.61	n.a.	0.00	n.a.	0.53	25.31
2011	CAMs	2.91	10.65	6.38	5.96	n.a.	0.00	n.a.	0.55	26.45
2012	CAMs	3.14	10.72	6.35	5.89	n.a.	0.00	n.a.	0.57	26.67
2013	CAMs	3.57	10.85	6.52	5.83	n.a.	0.00	n.a.	0.59	27.36
2014	CAMs	3.76	10.96	6.54	5.84	n.a.	0.01	n.a.	0.60	27.71
2015	CAMs	4.31	11.13	6.49	5.75	n.a.	0.01	n.a.	0.62	28.31
2016	CAMs	4.16	11.10	6.53	5.74	n.a.	0.00	n.a.	0.62	28.16
2017	CAMs	4.02	11.08	6.58	5.72	n.a.	0.00	n.a.	0.62	28.03
2018	CAMs	3.89	11.06	6.63	5.71	n.a.	0.00	n.a.	0.62	27.91
2019	CAMs	3.76	11.03	6.67	5.69	n.a.	0.01	n.a.	0.62	27.79
2020	CAMs	3.64	11.02	6.72	5.68	n.a.	0.01	n.a.	0.62	27.69
2008	CEDS	7.08	10.20	3.11	2.81	1.29	0.00	n.a.	0.03	24.53
2009	CEDS	5.91	11.07	3.15	3.45	1.33	0.00	n.a.	0.04	24.96
2010	CEDS	5.37	11.86	3.46	4.29	1.37	0.00	n.a.	0.05	26.40
2011	CEDS	5.06	12.61	3.75	4.56	1.22	0.00	n.a.	0.05	27.25
2012	CEDS	4.89	13.49	3.90	4.80	1.26	0.00	n.a.	0.05	28.40
2013	CEDS	4.85	13.32	4.08	4.84	1.25	0.00	n.a.	0.06	28.39
2014	CEDS	4.42	14.57	4.14	4.89	1.20	0.00	n.a.	0.06	29.29
2015	CEDS	4.69	13.61	4.23	4.95	1.34	0.00	n.a.	0.06	28.88
2016	CEDS	4.40	4.22	4.44	14.46	1.35	0.00	n.a.	0.06	28.93
2017	CEDS	4.10	13.94	4.66	4.87	1.35	0.00	n.a.	0.06	28.98

Table S11 continued from previous page

Year	emission inventories	transportation	residential	power	industry	agriculture	ships	aviation	waste	sum
2018	CEDS	3.79	13.88	4.68	4.89	1.36	0.00	n.a.	0.06	28.66
2019	CEDS	3.51	13.84	4.70	4.93	1.36	0.00	n.a.	0.06	28.39
2008	HTAP	6.24	11.58	0.07	3.35	2.01	0.03	0.00	0.50	23.79
2009	HTAP	6.36	12.30	0.07	3.58	2.07	0.04	0.00	0.53	24.95
2010	HTAP	6.41	13.13	0.09	3.98	2.12	0.04	0.00	0.55	26.33
2011	HTAP	6.68	14.23	0.10	4.24	1.89	0.04	0.00	0.58	27.77
2012	HTAP	6.77	14.97	0.10	4.44	1.97	0.05	0.00	0.60	28.91
2013	HTAP	6.67	15.70	0.11	4.65	1.94	0.05	0.00	0.62	29.73
2014	HTAP	6.76	16.47	0.10	4.80	1.87	0.06	0.00	0.64	30.70
2015	HTAP	6.71	16.42	0.10	4.90	1.89	0.05	0.00	0.66	30.73
2016	HTAP	6.18	16.69	0.11	5.05	2.06	0.05	0.00	0.68	30.82
2017	HTAP	5.96	17.07	0.11	5.24	2.04	0.06	0.00	0.70	31.18
2018	HTAP	5.30	17.81	0.13	5.60	2.03	0.06	0.00	0.71	31.65

S8 Identification of Key Sectors for Ozone Precursors Emission

Given the rapid changes in emissions and mitigated human activity in recent years in China, we need to identify the key sectors with fast shifts and diverse trends in total trend. We use the methodology introduced in section 2.2, step 1 of the main-body text. Table S12-Table S14 present the spreadsheet for calculation of trend assessment of integrated emission inventory for NO_x, CO and NMVOCs emissions.

Key sectors of NO_x emission indicated by integrated emission inventory are power (49% for trend contribution and -0.33 Tg yr⁻¹ for linear slope), industry (23% and 0.01 Tg yr⁻¹), ships (21% and 0.07 Tg yr⁻¹), as well as aviation (3% and 0.01 Tg yr⁻¹) in descending order. The trend contribution of these four sectors amounts to 95% collectively. Emerged sources, such as shipping and aviation, show an increasing trend and are opposite to the total emission trend. Key sectors of CO emission are industry (39% and -3.6 Tg yr⁻¹), residential (22% and -1.8 Tg yr⁻¹), power (13% and 0.14 Tg yr⁻¹), waste (13% and 0.15 Tg yr⁻¹), and transportation (11% and -1.0 Tg yr⁻¹). Key sectors of NMVOC emission are industry (50% and 0.65 Tg yr⁻¹), transportation (31% and -0.18 Tg yr⁻¹), and residential (18% and -0.11 Tg yr⁻¹).

The identification of key sectors ensures that three extra sectors we determined to be aggregated from global emission inventory (shipping, waste, and aviation) are particularly significant for emission inventory compilation. The aggregation level and breaking down of sectors adapted to IPCC suggestions (Intergovernmental Panel on Climate Change (IPCC), 2006). Therefore, aggregation of sectors reveals diverse changes and trends over years. The inclusion of three extra sectors from global emission inventory (shipping, waste, and aviation) implies the roles of missing sectoral emissions that cannot be ignored for ozone changes and emission inventory construction. These emission amounts require more attention regarding ozone mitigation.

Table S12. Trend assessment of integrated NO_x emission

Sectors	Precursors	Emission in 2008	Emission in 2020	Trend	Contribution	Cumulative Trend
power	NO _x	5.13	2.46	0.12	0.49	0.49
industry	NO _x	5.09	5.57	0.06	0.23	0.72
ships	NO _x	0.82	1.65	0.05	0.21	0.93
aviation	NO _x	0.06	0.16	0.01	0.03	0.95
waste	NO _x	0.16	0.24	0.01	0.02	0.98
residential	NO _x	0.64	0.52	0.00	0.01	0.99
agriculture	NO _x	0.19	0.21	0.00	0.01	1.00
transportation	NO _x	5.02	4.48	0.00	0.00	1.00

Table S13. Trend assessment of integrated CO emission

Sectors	Precursors	Emission in 2008	Emission in 2020	Trend	Contribution	Cumulative Total
industry	CO	79.99	45.23	0.05	0.39	0.39
residential	CO	69.80	52.40	0.03	0.22	0.62
power	CO	3.25	5.14	0.02	0.13	0.75
waste	CO	3.44	5.25	0.02	0.13	0.87
transportation	CO	32.42	19.54	0.01	0.11	0.98
ships	CO	0.29	0.58	0.00	0.02	1.00
aviation	CO	0.03	0.08	0.00	0.00	1.00
agriculture	CO	0.00	0.00	-	-	-

Table S14. Trend assessment of integrated NMVOC emission

Sectors	Precursors	Emission in 2008	Emission in 2020	Trend	Contribution	Cumulative Total
industry	NMVOC	11.34	18.31	0.21	0.50	0.50
transportation	NMVOC	6.57	4.23	0.13	0.31	0.81
residential	NMVOC	5.58	4.55	0.08	0.18	0.98
agriculture	NMVOC	1.29	1.36	0.00	0.01	0.99
ships	NMVOC	0.04	0.07	0.00	0.00	1.00
waste	NMVOC	0.03	0.06	0.00	0.00	1.00
power	NMVOC	0.06	0.06	0.00	0.00	1.00
aviation	NMVOC	0.00	0.00	0.00	0.00	1.00

S9 Sub-sectoral emissions of emission inventories

160 Figure S10 shows the changes in NO_x emissions from the six important sectors over the period 2008 to 2020. In the MEICv1.4 inventory, the electricity generation sector accounts for the largest amount of NO_x emissions, with an annual average of 6.3 Tg, or 26% of the total. In addition, transportation and industrial activities account for a large share: diesel vehicle (4.8 Tg, 19.9%), petrochemicals (2.5 Tg, 10.1%), Non-road mobile source (2.4 Tg, 10.0%), heating (2.4 Tg, 9.9%), and coking (1.7 Tg, 7.0%). For comparison with global emission inventories, we compared electricity generation in MEICv1.4 to the sum of electricity
165 public and autoproducer and other transformation (1A1a and 1A1bc) in CEDS and EDGAR emission inventories. MEIC and EDGAR NO_x emission from electricity generation (7.4 Tg and 6.3 Tg on annual average respectively) are higher than CEDS (5.4 Tg), but EDGARv6 has not declined as rapidly as MEIC and CEDS since 2012. The updated EDGARv8 inventory provides electricity generation (power) emission peaks earlier (in 2012) than previous versions, but the emission level still lower than the values of other inventories. For transportation sector, due to different sub-categories in MEIC emission inventory and global
170 EI, we have aggregated all transport-related sectors in each emission inventories for better comparison. In MEIC inventory, we mapped gasoline vehicles, diesel vehicles, motorcycle, and non-road mobile sources with transportation on the road (suggested by IPCC code 1A3b), on the rail (1A3c), and other transportation together in global CEDS and EDGAR inventories. NO_x emissions during transportation in MEIC emission inventory (7.7 Tg) are higher than global emission inventories (5.5 Tg). Leakage or release of NO_x during oil and gas storage and transportation can be up to 0.003 Tg, which has not been taken into
175 account in the emission inventory for MEIC. In addition, NO_x emissions from agricultural soil nitrogen fertilizers are integral (3D), with the global CEDS emission inventory reporting average annual emissions of 0.5 Tg for mainland China. The global EDGARv6 emission inventory reports that managing direct emissions of nitrous oxide (N₂O) from agricultural soils emits about 0.7 Tg of NO_x (3D).

Figure S13 shows differences of sectoral emission between existing emission inventories and integrated emission inventory
180 (emission of four existing emission inventories minus integrated inventory). For NO_x emission, CAMs emission inventory provides evidently lower emission comparing with integrated inventory, attributing to transportation (-2.2 Tg), shipping (-2.0 Tg), and waste emission (-0.3 Tg). And power generation emission and agriculture of global emission inventories take positive contribution (2.3 Tg) for the difference. The largest difference across emission inventories occurs in 2014. In EDGAR version 8, NO_x emissions peak earlier (in 2012) than in the previous version, as in MEIC and CEDS. However, the total values are
185 still lower than those of other inventories. Energy NO_x of EDGAR v8 mainly derives the changes over the years and the maximum value (about 9 Tg) occurs in 2011. Energy NO_x of previous EDGAR versions has no obvious changes over the years. Residential NO_x emissions for CEDS (MEIC) are the highest (lowest) of all inventories with an annual mean of 1.9 (0.9) Tg. Transport NO_x emissions (annual mean of 3.6 Tg) from edgarv6 (8) are closer to those from HTAP (4.3 Tg), but are still the lowest of all inventories.

190 Figure S11 shows the changes in inter-annual CO emission for mainland China (Tg) over the period 2008 to 2020 for six important sectors. The top six sectors in terms of average annual CO emissions and their percentages of the total are: coal combustion 36.7 Tg and 23.4%; coking 29.3 Tg and 18.7%; civilian biomass combustion 25.0 Tg and 18.7%, gasoline vehicle 22.3 Tg and 14.2%; other industries 15.9 Tg and 10%; petrochemical 6.9 Tg and 4.4%. Global CEDSv2021 CO from residential sector (68.8 Tg on annual average) are more in line with MEIC emission inventory (61.7 Tg) than EDGARv6
195 (31.9 Tg), and EDGAR residential CO emission has 50% underestimation comparing to MEIC and CEDS inventory. In the transportation sector, we similarly find that CEDS transportation CO emission (25.5 Tg on annual average) follow the same

trend as MEIC emission inventory (27.3 Tg) but are slightly higher than MEIC inventory, while EDGAR transportation CO emissions (5.1 Tg) are much lower than other emission inventories. In addition, we compare the subsectoral emissions of the two global inventories according to the definitions established by the IPCC: EDGAR underestimates the emissions from road transportation; And EDGARv6 overlooks oil and tanker transportation emission accounting as 0.3 Tg in CEDS inventory; In addition, neither MEICv1.4 nor EDGARv6 consider the waste sector (4A, 4B, 4C, 4D, and 4E in the IPCC codes), which in the CEDS emission inventory emits 5 Tg of CO; In both MEIC and CEDS, there is a rapid decrease in CO emissions from the metal production sector (2C), but in the EDGAR inventory (version 6 and 8), there is increasing variability.

For CO emission, CAMs emission inventory has large negative deviation from other emission inventories, ascribing to residential (-28.0 Tg), transportation (-8.8 Tg), and waste emission (-5.2 Tg). HTAP emission inventory has lower residential emission (-16.7 Tg), but it is counteracted by higher industry emission (16.3 Tg). And each year the two sectors change in the same proportion, which suggests a subsector is compiled in the industry sector of HTAP inventory, which in turn belongs to the residential sector of integrated inventory. The largest difference across emission inventories occurs in 2012. Agricultural CO emissions (biomass burning in agriculture) from EDGARv8 account for about 8 Tg, whereas the previous version did not include this sector for CO emissions. Transport CO emissions from EDGAR versions 6 and 8 appear to be lower (around 5 Tg) than other inventories (around 27 Tg). Transport NO_x emissions (annual average of 3.6 Tg) from EDGARv6 (8) are closer to those from HTAP (4.3 Tg), but are still the lowest of all inventories.

Figure S12 shows the changes in NMVOC emission over the period 2008-2020 for six important sectors. The top six sectors in terms of average annual NMVOC emissions and their percentages of the total are: industrial painting source 4.8 Tg and 18.4%; gasoline vehicles 3.9 Tg and 14.8%; civilian biomass combustion 2.9 Tg and 11.2%, iron and steel industry 2.8 Tg and 10.9%; other industries 12.8 Tg and 10.9%; architectural coating 1.4 Tg and 5.4%. One of the main contributors for NMVOCs emission is solvent source (2D, 2H, and 2L). We mapped the sum of industrial painting, printing and dyeing, architectural coatings and other industry source in MEICv1.4 to the sum of chemical-products-manufacture-processing source, paint application, and other process emission (2D), in global emission inventories (CEDSv2021 and EDGARv6). Solvent NMVOC emissions (2D) in the three emission inventories show an increasing trend, with linear slopes and annual averages of 0.5 Tg yr⁻¹ and 7.6 Tg, respectively, for MEICv1.4, 0.6 Tg yr⁻¹ and 10.1 Tg, respectively, for CEDSv2021, and 0.2 Tg yr⁻¹ and 7.8 Tg, respectively, for EDGARv6. MEICv1.4 ignores NMVOC emissions from agricultural activities, the total amount of which can be referred to the global emission inventories. According to CEDS recommendations, NMVOC emissions from fisheries are 0.4 Tg yr⁻¹.

For NMVOC emission, CAMs emission inventory still underestimates NMVOCs in residential (-8.8 Tg), industry (-8.8 Tg), agriculture (-8.8 Tg). CEDS has higher energy emission 4.6 Tg, and offset by negative industry emission by -4.5 Tg, which is from subsector fugitive emission. The industrial NMVOC emission of EDGARv8 has the highest values (16 Tg) compared to other inventories (15 Tg). Industry NMVOC emission of edgarv8 is lower than that in EDGARv6 by 2 Tg, which can be attributed to the missed sector in version 8 fugitive emission from soil fuel, and relatively lower (4.6 Tg) sector of production of solvent use than one (5.4 Tg) in EDGARv6. Industry NMVOC emission takes proportion about 60% of total emission, and derived the increasing trend of total values. EDGARv8 provides two more years of data suggesting a recovery after the COVID closure (2020). Residential NMVOC emissions (1A3 and 1A4) decreased in all inventories compared to 2008. HTAP provides the lowest values for NMVOC emissions in the residential sector with an annual average of 3.3 Tg. Road transport emissions account for the largest share of transport emissions in all global inventories, and road transport NMVOC emissions from EDGARv8 are slightly higher than those from version 6.

Emissions of CO and NO_x are well controlled in the major sources, with upward trends observed in all sources except heating sources. Among all sources, emissions from residential biomass combustion show a sharp downward trend, while emissions from residential chemical use exhibit an upward trend. The major sources of CO and NO_x emissions were mitigated around 2010 to 2013: CO emissions from coal combustion and industrial NO_x emissions from MEICv1.4 peaked in 2012, while the major sources of NMVOC emissions, such as industrial painting, dyeing and printing, and iron and steel production, peaked around 2018. NMVOC emissions are diverse and dispersed among many small and numerous sources, such as crafts and construction. Reducing NMVOC emissions remains challenging.

In summary, the changes in MEICv1.4 are consistent with China's timetable for implementing mitigation. CEDSv2021 incorporates the major sectors of the MEIC inventory, making CEDS similar to the changes in the MEIC inventory. However, the EDGAR data peaks a few years later than the former two, and the emissions are relatively low. Furthermore, CEDS provides more sectoral emissions data, such as waste CO emissions, agricultural soil NO_x emissions, etc., and offers a very detailed categorization based on official IPCC codes. This enhances our inter-comparison of key sectoral emissions in regional and global emission inventories and identifies sectors that emission inventories fail to notice. Full integration of sectoral emissions would therefore require an exhaustive comparison of all available emission indicators and the development of categorization criteria based on the IPCC report.



Figure S10. Interannual variation of top-6 important sectoral emissions for NO_x in mainland China from MEICv1.4, unit: Tg.

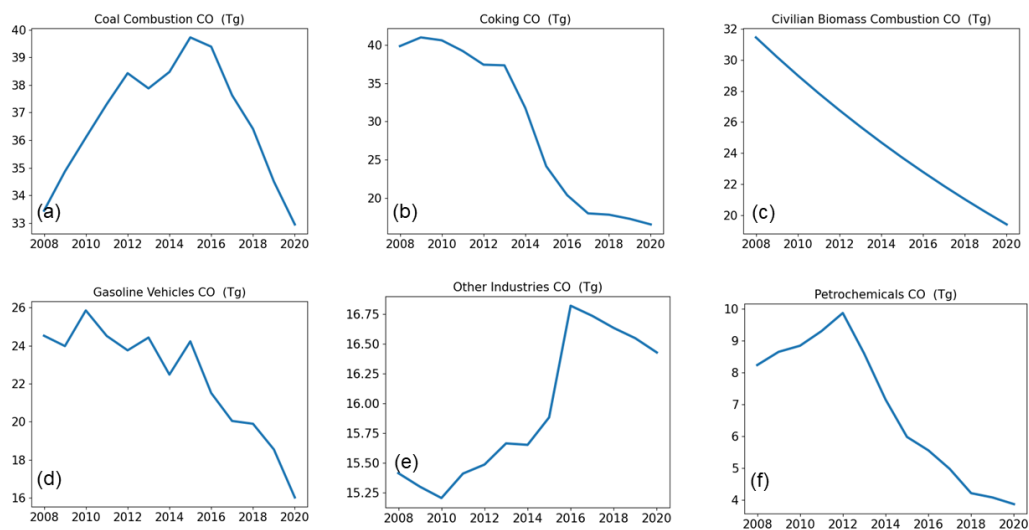


Figure S11. Same content with Figure S7, but for CO.

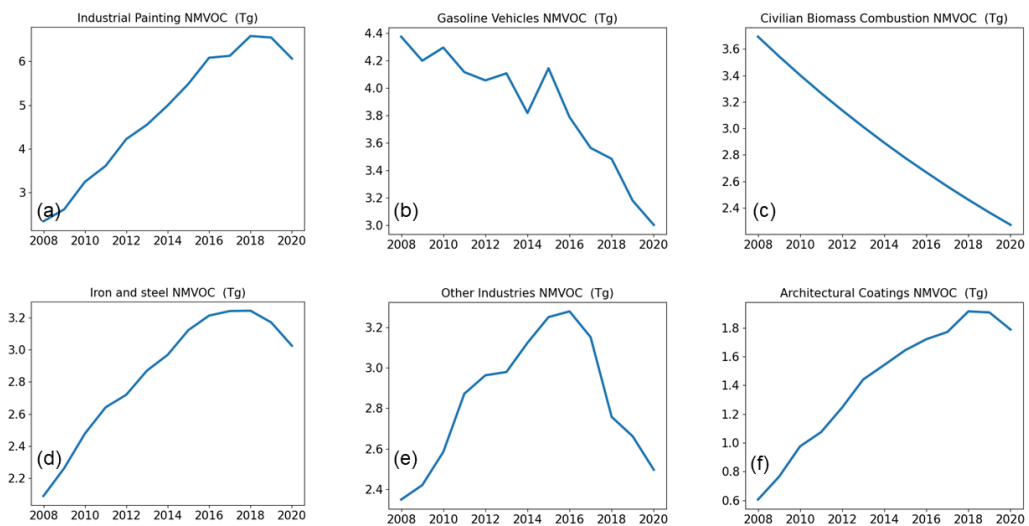


Figure S12. Same content with Figure S7, but for NMVOC.

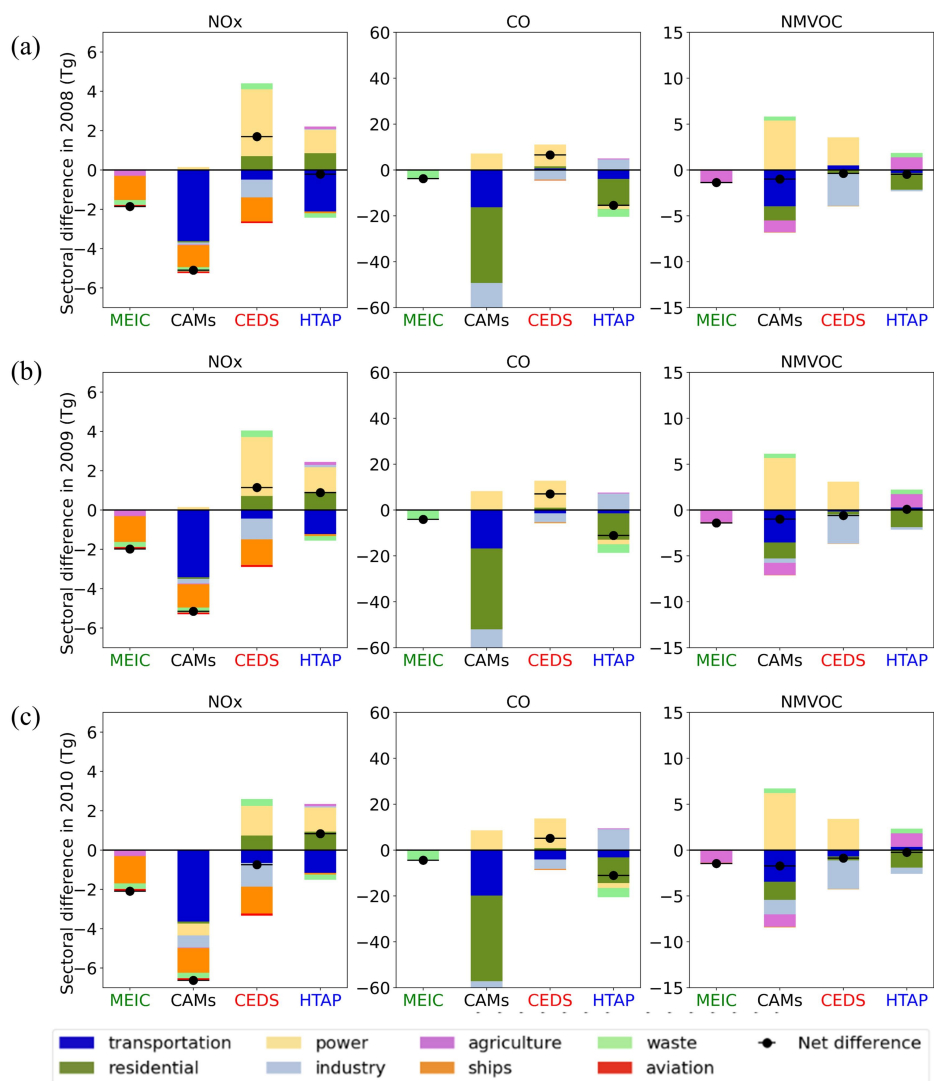


Figure S11. Differences of sectoral emissions over years from 2008 to 2010.

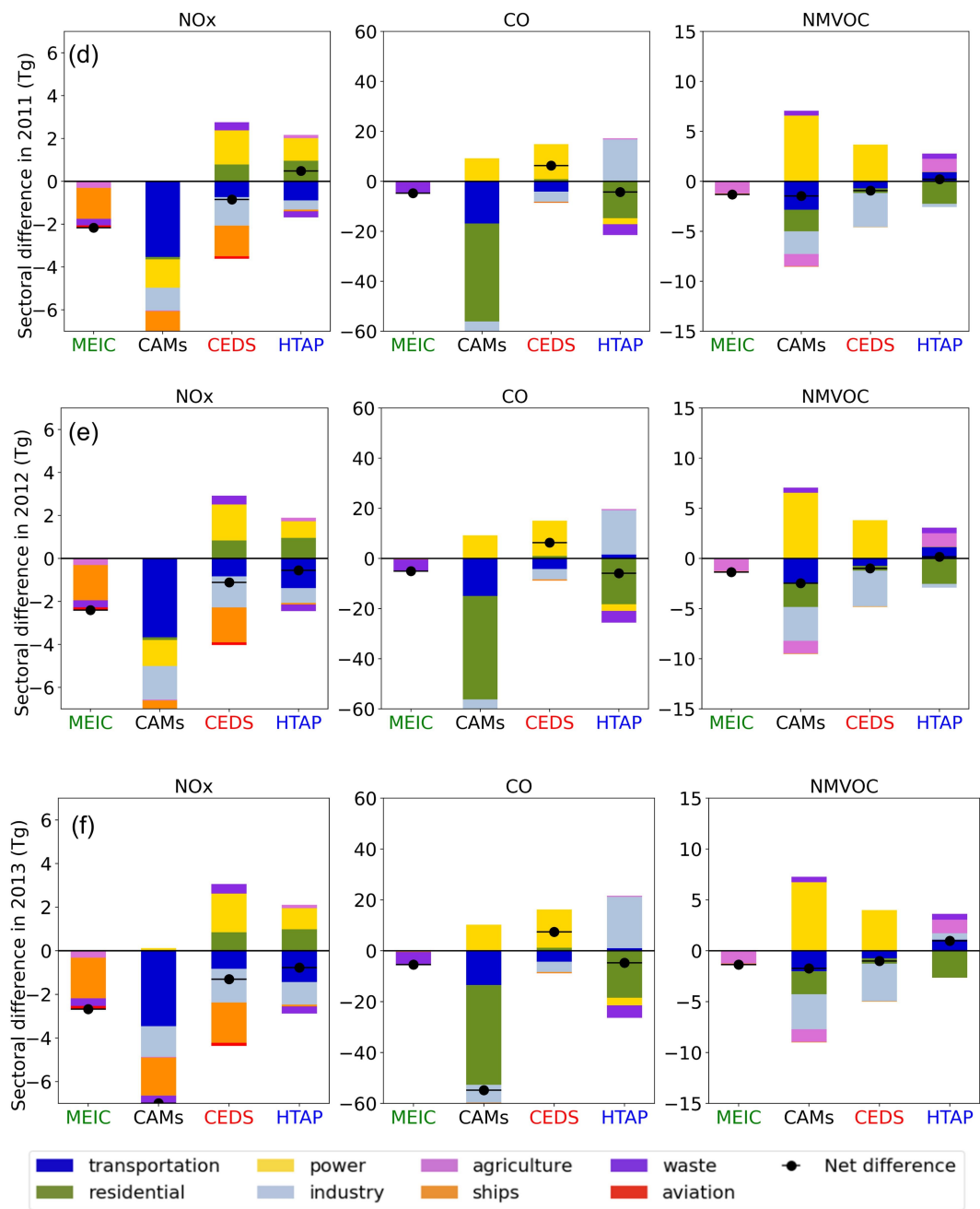


Figure S11. Differences of sectoral emissions over years from 2011 to 2013.

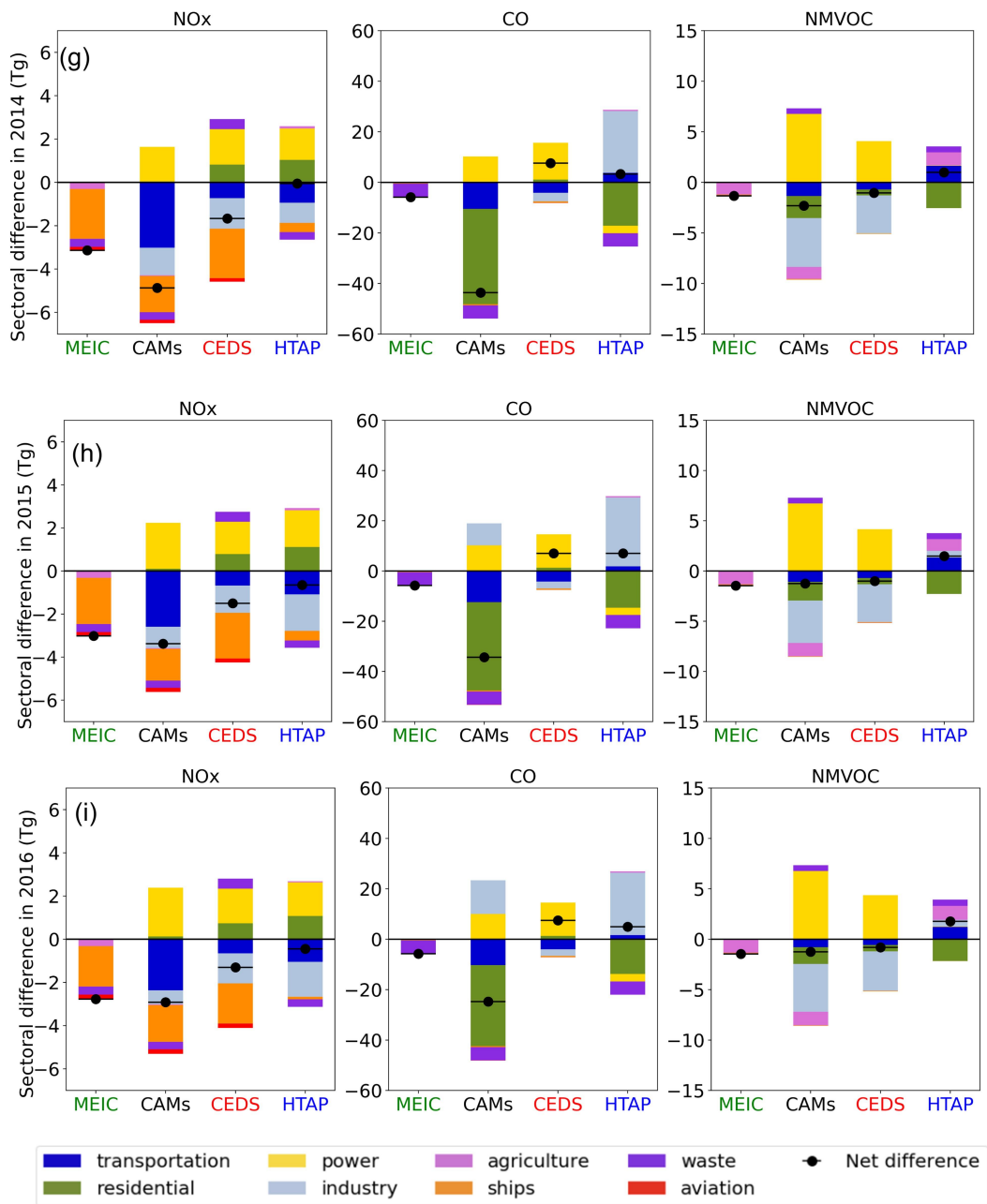


Figure S11. Differences of sectoral emissions over years from 2014 to 2016.

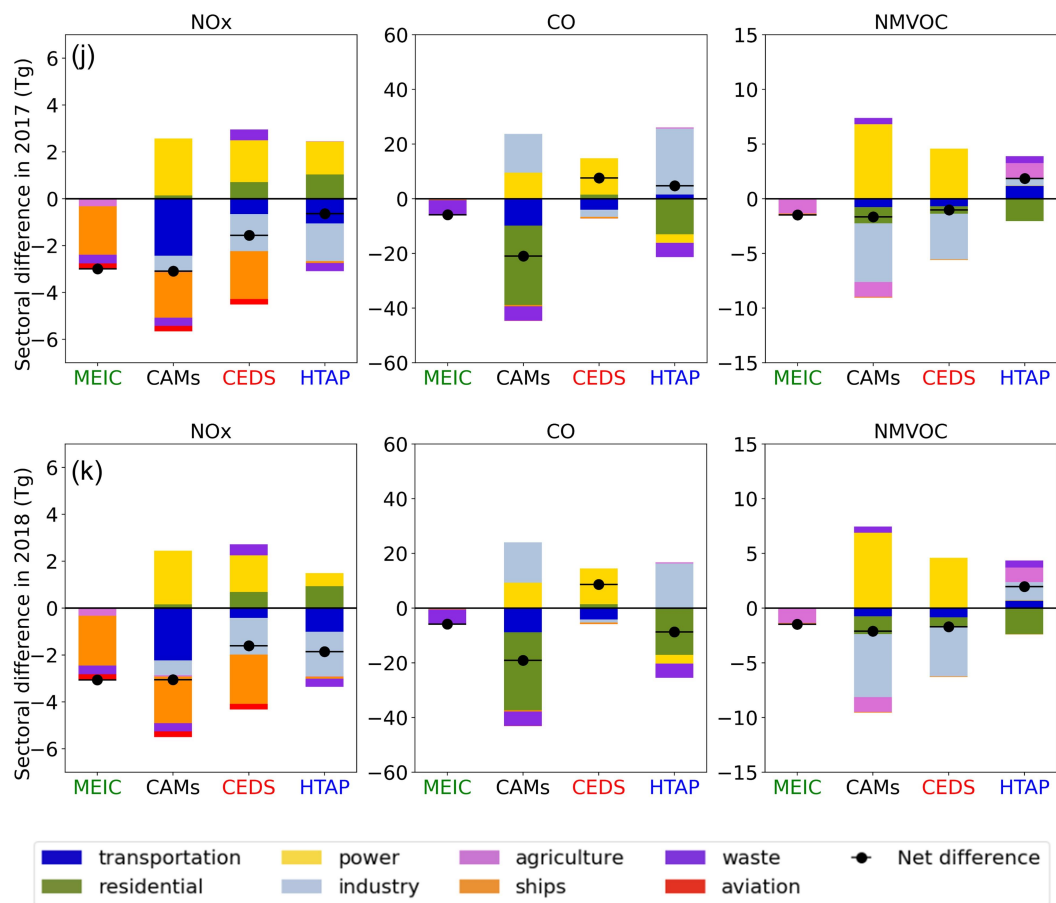


Figure S13. Differences of sectoral emissions over years from 2017 to 2018.

Table S15. Trends (Tg yr^{-1}) of CINEI sectoral emission for China over 2008 to 2020.

Sectors	NO_x	CO	NMVOCs
Power	-0.492 (± 0.079)***	0.147 (± 0.020)***	0.001 (± 0.001)
Industry	0.009 (± 0.064)	-3.588 (± 0.272)***	0.646 (± 0.084)***
Residential	-0.022 (± 0.004)***	-1.751 (± 0.203)***	-0.113 (± 0.016)***
Transportation	-0.049 (± 0.034)	-0.956 (± 0.094)***	-0.177 (± 0.009)***
Agriculture	0.005 (± 0.001)***	0.000 (± 0.000)	0.006 (± 0.004)
Waste	0.011 (± 0.002)***	0.151 (± 0.023)***	0.002 (± 0.000)***
Aviation	0.015 (± 0.001)***	0.005 (± 0.000)***	0.000 (± 0.000)***
Ships	0.102 (± 0.013)***	0.024 (± 0.002)***	0.003 (± 0.000)***
Sum	-0.421 (± 0.166)*	-5.969 (± 0.474)***	0.368 (± 0.090)***

Values in the table are calculated by linear slopes of sectoral emissions for mainland China, with standard deviations in parentheses. Slopes are marked with * if the p-value is in the range [0.05, 0.01], ** if in [0.01, 0.001], and *** if in [0.001, 0].

Table S16: Piece-wise slopes (Tg yr^{-1}) of CINEI for sectoral emissions that have an increasing trend followed by a decreasing trend.

Species	Sectors	Peak Year	Increasing Slope	Decreasing Slope
NO_x	Transportation	2012	0.21	-0.31
	Residential	2012	0.04	-0.04
	Power	2013	0.65	-0.79
	Industry	2013	0.87	-0.34
CO	Residential	2012	0.59	-2.44

The slopes in the table are calculated using piecewise linear regression. The period between 2008 and 2020 is divided into peak years. Therefore, the period in which the trends increase (decrease) is from 2008 (peak year) to the peak year (2020).

S10 Estimation of OFPs using integrated inventory (CINEI)

Figure S14 shows the integrated NMVOC emissions and OFPs composed of six NMVOC categories for the years 2008 to 2020. Individual NMVOC species are grouped into six main categories: alkanes, alkenes, alkynes, aromatics, oxygenated volatile organic compounds (OVOCs) and halocarbons. The integrated emission inventory shows the growth of NMVOC emissions and their OFPs. The total OFPs on annual averages are estimated at 115 Tg-O₃, with major contributions from aromatics (52 Tg-O₃, 45%), alkenes (34 Tg-O₃, 30%), OVOCs (11 Tg-O₃, 10%), and alkanes (8 Tg-O₃, 7%) (Figure S14). However, total NMVOC emissions in China have been estimated with a moderate uncertainty range of $\pm 68\%$ to $\pm 78\%$ (Zhang et al., 2009; Kurokawa et al., 2013), mainly due to the lack of reliable data for scattered areal sources. By examining the OFPs values within previous studies, as listed in Table S17, OFPs are mainly composed of aromatics and alkenes. The OFPs of alkenes and OVOCs from integrated emission inventory are relatively higher than those in (Li et al., 2019), which could be attributed to the aggregated sectors (such as agriculture) and additional species from the updated speciated profiles, such as halocarbons, as well as a larger fraction of highly reactive species, including alkenes (Mo et al., 2016).

Industry (approximately 65%), transportation (approximately 11%), and residential (approximately 20%) sectors mainly compose the key NMVOCs emission. Furthermore, agriculture is an inevitable sector for some alkene or alkyne species, like ethene (approximately 12%), propene (approximately 2%), and ethyne (approximately 4%), since diesel vehicles used for fishing and harvesting emit signature olefins. However, this remarkable contribution is overlooked by national inventories. In addition, we first speciate waste and aviation NMVOC emissions for China, which are left out from regional emission inventories. Waste emission traces back to incineration and open burning of waste, and handling of liquid wastes and sludge from industrial processes, and chiefly involves ethene (0.01 Tg), formaldehyde (0.007 Tg), and acetaldehyde (0.007 Tg). Chemicals of aviation and ships emission include alkenes and alkanes at a negative 3rd to 4th power of 10 Tg. Industry, transportation, and residential sectors are the main sectors of NMVOCs emission. This suggests that scenarios with different VOCs speciation impact ozone formation differently, and mitigation policies should pay more attention to controlling highly reactive species such as xylene, ethene, and toluene, especially regarding aromatics, where solvent usage was the most important contributor to toluene and m,p-xylene in the Zheng's emission inventory.

Based on the VOC emissions analysis from 2008-2020, the overall increase in Ozone Formation Potential (OFP) of 1.3% annually was primarily driven by significant growth in industrial emissions, which increased by 3.9% per year across most VOC species. This industrial growth more than compensated for the decreasing trends in transportation (-3.3% annually) and residential (-2.2% annually) sectors. The species contributing most to ozone formation—m/p-Xylene (17.7% of total OFP), Propene (16.7%), and Toluene (10.0%)—all showed increasing industrial emissions despite reductions from other sectors (Figures S15 and S16).

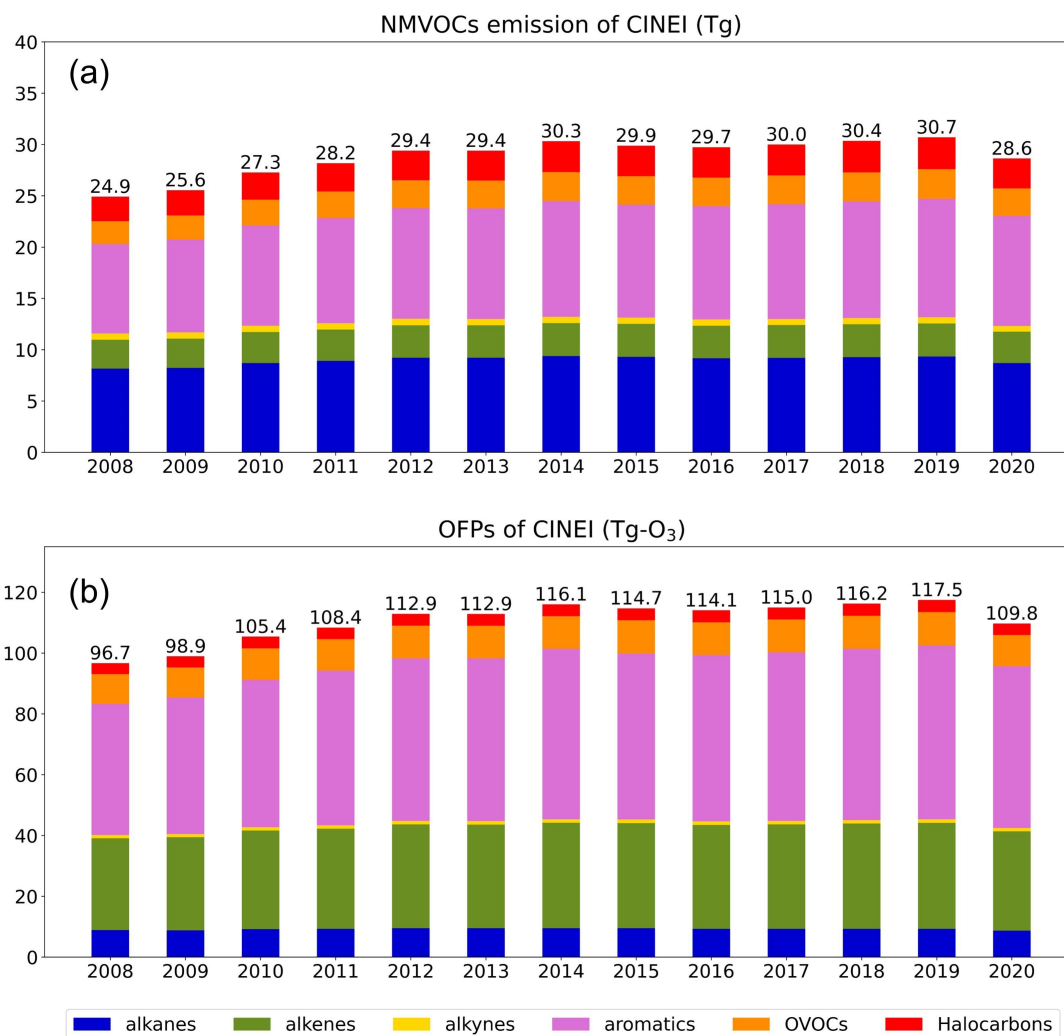


Figure S14. Inter-annual NMVOCs variations of Integrated Emissions for China during 2008 to 2020. (a) Emissions of six NMVOCs groups: alkanes, alkenes, alkynes, aromatics, OVOCs, and halocarbons (Unit: Tg). (b) OFPs of six NMVOCs groups (Unit: Tg-O₃).

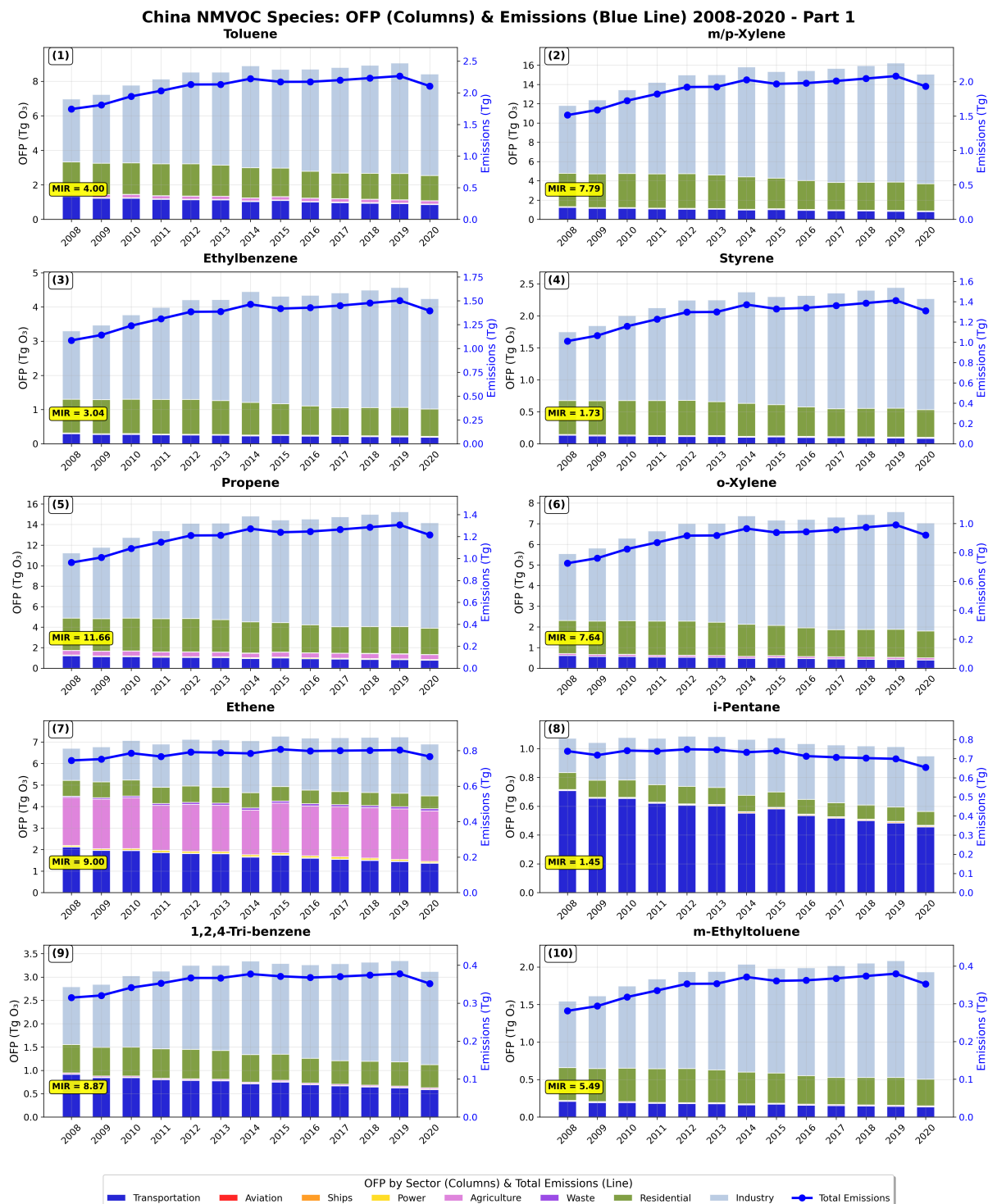


Figure S15. Year-to-year CINEI Ozone formation potentials (OFPs, in columns, unit: Tg per year) and emission (black line with dots, unit: Tg) for the TOP-20 important NMVOC species in China from 2008 to 2020. The colors of the columns denote sectors' contribution to OFP.

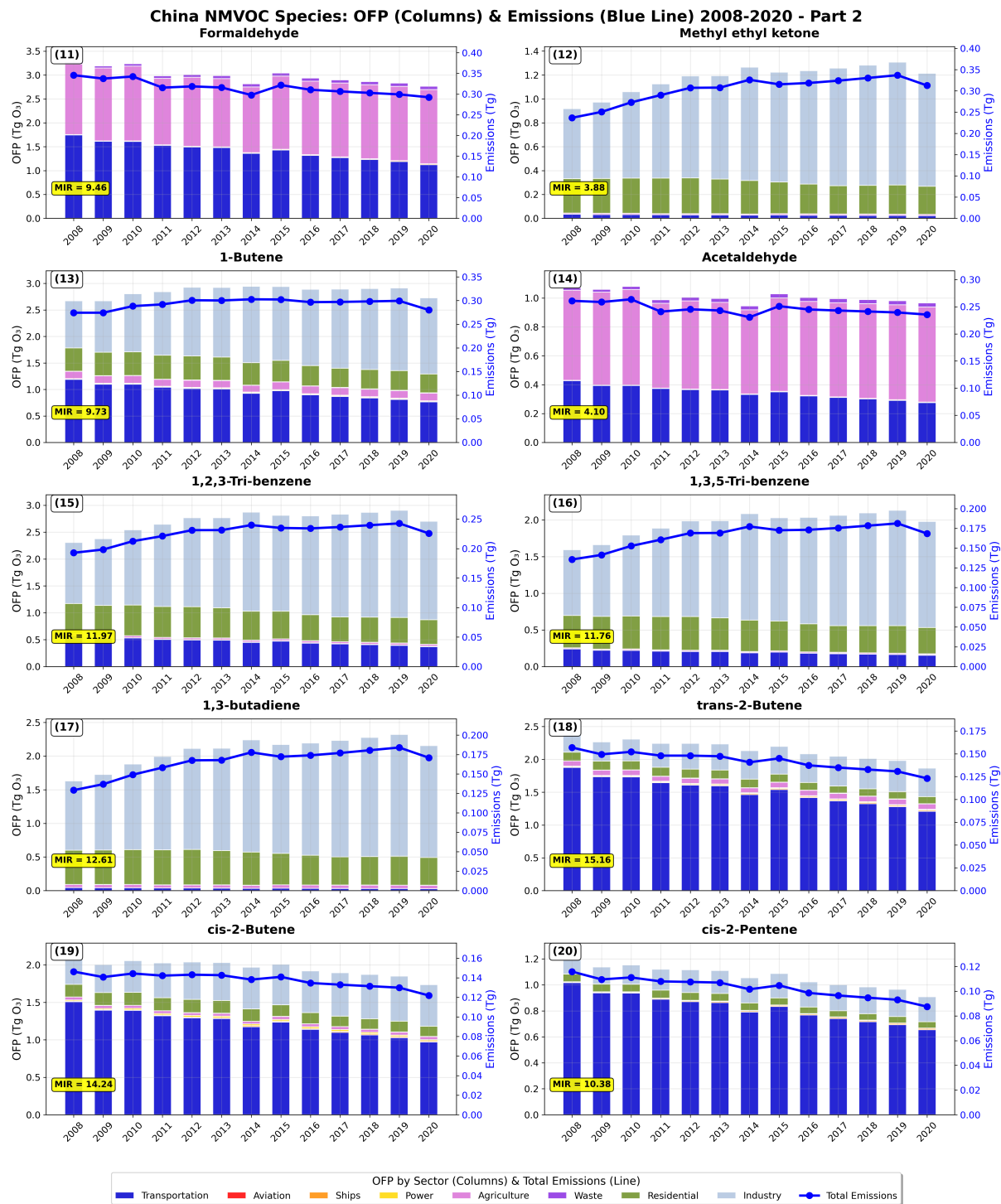


Figure S16. Year-to-year CINEI Ozone formation potentials (OFPs, in columns, unit: Tg-O₃) and emission (black line with dots, unit: Tg) for the TOP-20 important NMVOC species in China from 2008 to 2020. The colors of the columns denote sectors' contribution to OFP.

Table S17: OFP comparisons with literatures

Literatures/This study	Period	Region	Total (Tg-O ₃)	Alkanes	Alkenes	Alkynes	Aromatics	OVOCs
Li et al. (2019)	2017	China	99.7	8.00%	37.00%	0.01%	43.00%	10.00%
This study	2017	China	106.2	8.03%	40.2%	0.41%	39.3%	12.00%
Ou et al. (2015)	2010	PRD_cities	n.a.	9.6%	25.8%	n.a.	59.4%	5.1%
This study	2010	PRD_cities	2.33	9.44%	44.82%	0.94%	35.79%	8.99%
Wu and Xie (2017)	2013	NCP	26.8	9.2%	30.3%	n.a.	40.8%	n.a.
This study	2013	NCP	27.3	8.11%	45.54%	0.87%	36.83%	8.66%
Wu and Xie (2017)	2013	YZR	18.48	7.3%	24.7%	n.a.	50.00%	n.a.
This study	2013	YZR	12.86	8.16%	46.9%	0.91%	36.16%	7.86%
Wu and Xie (2017)	2013	PRD	9.36	8.1%	22.8%	n.a.	54.8%	n.a.
This study	2013	PRD	5.11	8.55%	47.59%	0.98%	34.02%	8.86%
Liang et al. (2020)	2018	Nanjing	n.a.	10.3%	19.1%	n.a.	64.1%	6.5%
This study	2018	Nanjing	0.83	7.80%	31.54%	0.37%	49.89%	10.4%

The values in the table are the total OFPs for the regions and the percentages of the VOC groups with respect to the total OFPs. In order to guarantee comparability, we specify the regions according to the definition in the literature. In particular, Pearl River Delta cities (PRD_cities) include the cities of Shenzhen, Zhuhai, Dongguan, Jiangmen, Foshan, Zhongshan, Zhaoqing and Huizhou. North China Plain (NCP) includes the municipalities of Beijing and Tianjin and the provinces of Hebei, Shandong and Henan. The Yangtze River Delta includes the municipality of Shanghai and the provinces of Jiangsu and Zhejiang. PRD represents Guangdong Province. n.a. indicates that the value is not available in the literature.

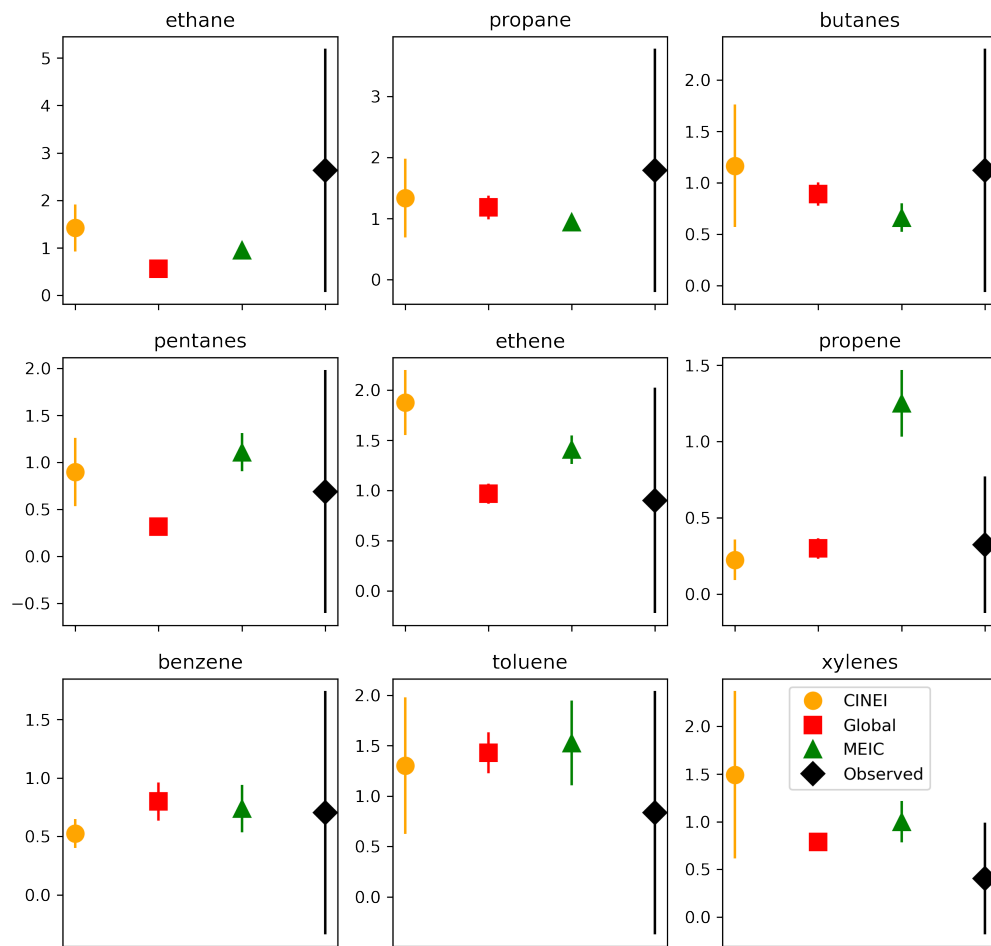


Figure S17. Comparisons of ratios of 9 species to C_2H_2 of integrated inventory (CINEI), national MEIC inventory, global inventories, and observed ratios (mol/mol). The VOC measurement data is listed in the following table.

Table S18. VOC mixing ratios (ppbv) from in situ-measurement in literatures

species	Langfang ^a	Nanjing_NUIST ^b	Nanjing_PAES ^b	Nanjing_ZJS ^b	Nanjing_NJU ^b
ethane	6.83±7.5	6.56±8.13	6.19±5.93	6.13±8.92	3.98±2.31
propane	7.05±6.55	4.13±2.63	4.26±2.30	4.12±2.22	3.08±0.97
butane	4.09±4.03	3.32±1.27	2.91±0.66	3.35±1.34	3.95±1.94
pentanes	1.92±1.62	1.06±0.56	1.00±0.41	1.07±1.08	3.12±1.82
ethene	1.25±0.92	n.a.	1.95±2.12	1.88±1.74	1.19±0.43
propene	0.68±0.45	n.a.	n.a.	1.54±3.44	1.92±2.91
benzene	0.86±0.63	1.33±1.68	0.91±0.67	1.01±1.33	n.a.
toluene	0.84±0.63	1.31±1.56	1.14±1.26	1.13±1.55	1.29±3.14
xylenes	0.69±0.64	n.a.	n.a.	n.a.	n.a.
acetylene	4.91±5.7	2.37±1.27	2.65±1.99	2.18±0.99	2.42±1.80
species	Nanjing_GCH ^b	Beijing ^c	GC ^d	QZ ^d	Wuhan
ethane	4.55±6.30	4.37±1.65	4.43±1.93	3.53±1.51	3.91±2.18
propane	3.65±2.45	2.44±1.57	2.61±1.65	1.94±1.12	5.49±6.64
butane	3.11±1.18	2.46±1.87	2.64±1.94	0.59±0.46	1.74±0.26
pentanes	0.94±0.37	1.55±1.12	1.07±0.82	1.1±1.55	0.44±0.37
ethene	1.73±1.55	2.33±1.58	3.04±2.39	1.92±1.61	1.97±1.61
propene	0.79±0.25	n.a.	0.84±1.66	n.a.	0.43±0.46
benzene	0.90±1.47	0.82±0.52	1.08±0.68	0.81±0.48	0.49±0.28
toluene	1.63±2.00	1.33±1.12	1.31±1.46	0.48±0.35	0.71±0.63
xylenes	n.a.	n.a.	n.a.	n.a.	0.27±0.03
acetylene	2.18±1.22	2.17±1.42	2.45 ± 1.66	1.94±1.12	1.80±0.03
species	PRD ^e	Beijing_BNU ^c	Guilin	Zhengzhou	Weinan
ethane	3.86±1.34	5.31±3.2	1.29±0.73	4.37±1.91	3.94±1.877
propane	3.01±1.82	4.18±3.18	1.05±0.60	2.32±1.11	3.498±1.854
butane	1.85±1.28	3.31±2.69	0.55±0.38	1.73±1.41	3.133±2.271
pentanes	1.9±2.2	1.58±1.46	0.24±0.23	0.83±0.66	2.90±3.66
ethene	2.94±3.34	3.74±4.34	0.65±0.44	1.31±0.77	1.421±0.918
propene	n.a.	0.94±1.22	0.16±0.10	0.23±0.15	0.290±0.193
benzene	n.a.	0.92±0.87	2.92±1.84	0.62±0.32	0.467±0.386
toluene	3.74±2.89	0.98±0.92	4.20±3.20	0.93±1	0.751±0.839
xylenes	1.62±1.44	0.6±0.66	0.94±1.18	n.a.	0.742±1.126
acetylene	3.42±2.33	3.126±3.43	0.75±0.57	1.51±0.79	2.252±1.686

species	Shanghai	Handan	Chengdu	Chongqing_CJZ ^d	Chongqing_CQ ^d
ethane	3.69±2.03	5.53±3.22	7.70±3.87	5.5±1.6	5.2±1.6
propane	3.01±2.20	4.05±3.10	3.23±3.86	1.4±0.6	3.3±4.0
butane	2.48±1.99	1.82±1.50	3.07±7.29	1.1±0.5	1.4±1
pentanes	1.58±1.29	1.09±1.00	4.23±3.36	0.8±0.5	1.4±1.2
ethene	1.53±1.23	1.18±1.31	3.84±3.07	3.9±2	3±1.8
propene	0.49±0.64	0.40±0.28	0.85±0.90	0.8±0.5	0.6±0.4
benzene	0.42±0.27	1.87±2.58	1.41±1.56	1.1±0.5	1.0±0.5
toluene	1.31±1.28	1.49±1.47	1.93±4.8	1.2±0.7	0.8±0.6
xylenes	1.52±0.98	0.98±1.19	1.15±2.95	0.7±0.6	0.9±1.2
acetylene	1.2±0.87	0.33±0.20	4.29±3.32	4.5±3	3.9±2.4

Some cities include more than one observed site, so we average the values of all observed sites in a city to represent the value in the city.

a. is marked as sites in Langfang city; b. in Nanjing city; c. in Beijing city; d. in Xiamen city; e. in Heshan city.

Table S19. Information of in-situ measurement of NMVOC species mixing ratios in literatures.

sites	latitude (°)	longitude (°)	date_start (yyyy-mm)	date_end	type	city	province	references
Langfang	40	116.5	2016-04	2017-03	urban	langfang	hebei	(Lv et al., 2021)
Zhengzhou	34.75	113.60	2020-09	2020-09	urban	zhengzhou	henan	(Huang et al., 2022)
Handan	36.57	114.5	2018-05	2018-06	urban	handan	hebei	(Yao et al., 2021)
Weinan	34.488	109.497	2019-08	2019-09	urban	weinan	shanxi	(Hui et al., 2021)
Beijing	39.9	116.4	2018-01	2018-12	urban	beijing	beijing	(Li et al., 2022a, 2022b)
Guilin	25.2	110.2	2018-05	2018-11	urban	guilin	guangxi	(Zhang et al., 2019)
Xi'an	34.3	109.01	2019-06	2019-07	urban	xi'an	shanxi	(Song et al., 2021)
Xiamen	24.28	118.09	2016-08	2016-12	urban	xiamen	fujian	(Hong et al., 2019)
Chengdu	30.6	104	2016-05	2017-01	urban	chengdu	sichuan	(Simayi et al., 2020)
Shanghai	31.2	121.5	2017-05	2017-05	urban	shanghai	shanghai	(Li et al., 2022b)
Guangzhou	23	113.21	2011-06	2012-05	urban	guangzhou	guangdong	(Zou et al., 2015)
Heshan	22.728	112.93	2014-10	2014-11	rural	jiangmen	guangdong	(He et al., 2019)
Nanjing	32.1	118.4	2018-07	2018-08	urban	nanjing	jiangsu	(Mozaffar et al., 2020)
Wuhan	30.54	114.36	2017-05	2017-05	urban	wuhan	hubei	(Hui et al., 2020a)
Chongqing	29.83	106.28	2015-07	2015-08	urban	chongqing	chongqing	(Hui et al., 2020b)
Taiwan	23.6	120.2	2014-01	2016-12	urban	taixin	taiwan	(Chen et al., 2019)

Table S20: Emission of individual NMVOC species based on integrated emission and source profiles for annual average of 2008-2020 (Unit: Tg).

Species	transportation	aviation	ships	power	agriculture	waste	residential	industry
Ethane	3,79E-02	1,84E-05	3,76E-04	1,22E-02	8,44E-02	3,40E-03	1,29E-01	4,11E-01
Propane	2,24E-01	1,09E-04	2,22E-03	4,64E-03	1,36E-02	5,48E-04	1,98E-01	6,33E-01
i-Butane	1,29E-01	6,28E-05	1,28E-03	0,00E+00	2,45E-03	9,86E-05	1,12E-01	3,57E-01
n-Butane	1,73E-01	8,39E-05	1,71E-03	4,40E-04	5,20E-03	2,10E-04	1,11E-01	3,56E-01
Cyclopentane	1,83E-02	8,85E-06	1,81E-04	0,00E+00	0,00E+00	0,00E+00	1,29E-02	4,14E-02
i-Pentane	3,96E-01	1,92E-04	3,93E-03	7,71E-04	1,53E-03	6,16E-05	7,60E-02	2,43E-01
n-Pentane	1,84E-01	8,91E-05	1,82E-03	9,66E-04	3,36E-03	1,36E-04	6,62E-02	2,12E-01
Methylcyclopentane	4,86E-02	2,36E-05	4,82E-04	1,87E-04	0,00E+00	0,00E+00	2,36E-02	7,55E-02
Cyclohexane	1,44E-02	6,98E-06	1,43E-04	9,37E-05	0,00E+00	0,00E+00	2,78E-02	8,90E-02
2,2-Dimethylbutane	2,30E-02	1,12E-05	2,28E-04	0,00E+00	2,62E-04	1,06E-05	5,19E-03	1,66E-02
2,3-Dimethylbutane	5,38E-02	2,61E-05	5,33E-04	8,65E-05	3,50E-04	1,41E-05	8,88E-03	2,84E-02
2-Methylpentane	1,67E-01	8,12E-05	1,66E-03	4,25E-04	8,74E-04	3,52E-05	3,76E-02	1,20E-01
3-Methylpentane	1,20E-01	5,84E-05	1,19E-03	1,30E-04	9,18E-04	3,70E-05	3,15E-02	1,01E-01
n-Hexane	4,93E-02	2,39E-05	4,89E-04	7,06E-04	4,15E-03	1,67E-04	8,10E-02	2,59E-01
Methylcyclohexane	2,13E-02	1,03E-05	2,11E-04	6,49E-05	0,00E+00	0,00E+00	2,28E-02	7,30E-02
2,3-Dimethylpentane	1,93E-02	9,37E-06	1,92E-04	2,31E-04	0,00E+00	0,00E+00	9,16E-03	2,93E-02
2,4-Dimethylpentane	1,32E-02	6,41E-06	1,31E-04	0,00E+00	0,00E+00	0,00E+00	2,00E-03	6,38E-03
2-Methylhexane	5,84E-02	2,83E-05	5,79E-04	9,37E-05	6,99E-04	2,82E-05	2,99E-02	9,57E-02
3-Methylhexane	5,10E-02	2,47E-05	5,05E-04	0,00E+00	6,12E-04	2,46E-05	2,63E-02	8,43E-02
n-Heptane	4,14E-02	2,01E-05	4,10E-04	8,51E-04	7,34E-03	2,96E-04	4,35E-02	1,39E-01
2,2,4-Trimethylpentane	3,99E-02	1,94E-05	3,96E-04	0,00E+00	4,37E-05	1,76E-06	3,23E-03	1,03E-02
2,3,4-Trimethylpentane	1,73E-02	8,39E-06	1,71E-04	0,00E+00	0,00E+00	0,00E+00	2,65E-03	8,47E-03
2-Methylheptane	1,91E-02	9,27E-06	1,89E-04	3,39E-04	0,00E+00	0,00E+00	1,37E-02	4,38E-02
3-Methylheptane	1,54E-02	7,49E-06	1,53E-04	1,23E-04	0,00E+00	0,00E+00	1,09E-02	3,48E-02
n-Octane	3,80E-02	1,84E-05	3,77E-04	5,98E-04	1,14E-03	4,58E-05	3,64E-02	1,16E-01
n-Nonane	2,09E-02	1,01E-05	2,07E-04	3,46E-04	0,00E+00	0,00E+00	3,72E-02	1,19E-01
n-Decane	2,27E-02	1,10E-05	2,25E-04	3,89E-04	0,00E+00	0,00E+00	3,58E-02	1,15E-01
n-Un.a.cecane	7,36E-02	3,57E-05	7,30E-04	3,75E-04	0,00E+00	0,00E+00	3,50E-02	1,12E-01
Ethene	1,91E-01	9,26E-05	1,89E-03	9,20E-03	2,51E-01	1,01E-02	7,63E-02	2,44E-01
Propene	8,43E-02	4,09E-05	8,36E-04	6,47E-03	3,90E-02	1,57E-03	2,52E-01	8,06E-01

Table S20 continued from previous page

Species	transportation	aviation	ships	power	agriculture	waste	residential	industry
1,3-butadiene	2,88E-03	1,40E-06	2,86E-05	0,00E+00	3,76E-03	1,51E-04	3,77E-02	1,21E-01
1-Butene	9,92E-02	4,81E-05	9,83E-04	1,07E-03	1,42E-02	5,72E-04	4,21E-02	1,35E-01
cis-2-Butene	8,59E-02	4,17E-05	8,52E-04	1,34E-03	2,71E-03	1,09E-04	1,11E-02	3,56E-02
trans-2-Butene	1,00E-01	4,87E-05	9,96E-04	7,43E-04	5,24E-03	2,11E-04	8,19E-03	2,62E-02
Isoprene	9,73E-03	4,72E-06	9,65E-05	0,00E+00	9,48E-03	3,82E-04	5,80E-03	1,85E-02
1-Pentene	4,30E-02	2,09E-05	4,26E-04	5,19E-04	1,49E-03	5,99E-05	1,35E-02	4,30E-02
cis-2-Pentene	7,94E-02	3,85E-05	7,87E-04	6,49E-05	1,75E-04	7,04E-06	5,30E-03	1,70E-02
trans-2-Pentene	5,04E-02	2,45E-05	5,00E-04	5,05E-05	2,67E-03	1,07E-04	4,85E-03	1,55E-02
1-Hexene	2,18E-02	1,06E-05	2,16E-04	3,89E-04	1,75E-04	7,04E-06	1,16E-02	3,72E-02
Ethylene	2,47E-01	1,20E-04	2,45E-03	4,40E-03	8,01E-02	3,23E-03	2,07E-02	6,63E-02
Benzene	1,37E-01	6,66E-05	1,36E-03	1,18E-02	1,05E-01	4,24E-03	8,62E-02	2,76E-01
Toluene	2,69E-01	1,30E-04	2,67E-03	5,33E-03	4,56E-02	1,84E-03	4,20E-01	1,34E+00
m/p-Xylene	1,29E-01	6,24E-05	1,28E-03	1,62E-03	7,52E-03	3,03E-04	4,16E-01	1,33E+00
Ethylbenzene	7,88E-02	3,82E-05	7,82E-04	6,49E-04	6,20E-03	2,50E-04	3,03E-01	9,70E-01
o-Xylene	6,51E-02	3,16E-05	6,45E-04	5,77E-04	1,17E-02	4,72E-04	1,96E-01	6,26E-01
Styrene	6,21E-02	3,01E-05	6,16E-04	3,60E-05	7,47E-03	3,01E-04	2,87E-01	9,18E-01
1,2,3-Trimethylbenzene	3,90E-02	1,89E-05	3,87E-04	1,59E-04	2,84E-03	1,14E-04	4,38E-02	1,40E-01
1,2,4-Trimethylbenzene	8,34E-02	4,05E-05	8,28E-04	2,67E-04	2,88E-03	1,16E-04	6,44E-02	2,06E-01
1,3,5-Trimethylbenzene	1,65E-02	8,02E-06	1,64E-04	9,37E-05	1,22E-03	4,93E-05	3,52E-02	1,12E-01
i-Propylbenzene	2,06E-02	9,99E-06	2,04E-04	1,44E-05	1,75E-04	7,04E-06	1,92E-02	6,13E-02
m-Ethyltoluene	3,07E-02	1,49E-05	3,05E-04	2,09E-04	1,88E-03	7,57E-05	7,46E-02	2,39E-01
n-Propylbenzene	7,75E-02	3,76E-05	7,68E-04	5,77E-05	8,74E-04	3,52E-05	2,48E-02	7,92E-02
o-Ethyltoluene	4,52E-02	2,19E-05	4,48E-04	1,01E-04	3,50E-04	1,41E-05	2,62E-02	8,38E-02
p-Ethyltoluene	2,16E-02	1,05E-05	2,15E-04	9,37E-05	6,99E-04	2,82E-05	2,67E-02	8,53E-02
m-Diethylbenzene	3,18E-02	1,54E-05	3,16E-04	6,49E-05	0,00E+00	0,00E+00	7,73E-03	2,47E-02
p-Diethylbenzene	2,10E-02	1,02E-05	2,08E-04	1,80E-04	0,00E+00	0,00E+00	1,67E-02	5,35E-02
tetrachloromethane	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	1,33E-02	4,26E-02
Chloroform	2,18E-04	1,06E-07	2,16E-06	0,00E+00	0,00E+00	0,00E+00	1,27E-02	4,07E-02
Dichloromethane	0,00E+00	0,00E+00	0,00E+00	0,00E+00	2,40E-03	9,68E-05	1,54E-01	4,94E-01
Chloromethane	0,00E+00	0,00E+00	0,00E+00	0,00E+00	1,04E-02	4,17E-04	3,24E-02	1,04E-01
Tetrachloroethylene	2,42E-05	1,17E-08	2,40E-07	0,00E+00	0,00E+00	0,00E+00	4,08E-03	1,30E-02

Table S20 continued from previous page

Species	transportation	aviation	ships	power	agriculture	waste	residential	industry
Vinyl chloride	2,42E-05	1,17E-08	2,40E-07	0,00E+00	0,00E+00	0,00E+00	2,03E-01	6,51E-01
Formaldehyde	1,50E-01	7,26E-05	1,48E-03	0,00E+00	1,58E-01	6,38E-03	0,00E+00	0,00E+00
Acetaldehyde	8,45E-02	4,10E-05	8,38E-04	0,00E+00	1,55E-01	6,23E-03	0,00E+00	0,00E+00
acrolein	1,45E-02	7,02E-06	1,44E-04	0,00E+00	1,04E-02	4,17E-04	0,00E+00	0,00E+00
Methanol	7,05E-03	0,00E+00	1,43E-05	0,00E+00	7,98E-02	0,00E+00	3,88E-02	5,23E-03
Ethanol	5,68E-06	0,00E+00	7,87E-05	0,00E+00	4,52E-01	0,00E+00	2,97E-02	8,29E-02
Propionaldehyde/Propanal	2,37E-02	1,15E-05	2,35E-04	0,00E+00	3,03E-02	1,22E-03	0,00E+00	0,00E+00
Butyraldehyde/n-Butanal	2,84E-02	1,38E-05	2,81E-04	0,00E+00	1,26E-02	5,07E-04	0,00E+00	0,00E+00
Valeraldehyde/n-Pentanal	7,99E-03	3,88E-06	7,92E-05	0,00E+00	1,26E-02	5,09E-04	0,00E+00	0,00E+00
Isovaleraldehyde	8,26E-03	4,00E-06	8,19E-05	0,00E+00	6,51E-03	2,62E-04	0,00E+00	0,00E+00
Benzaldehyde	1,41E-02	6,83E-06	1,40E-04	0,00E+00	1,48E-02	5,95E-04	0,00E+00	0,00E+00
Hexanaldehyde/n-Hexanal	1,39E-02	6,75E-06	1,38E-04	0,00E+00	1,97E-02	7,92E-04	0,00E+00	0,00E+00
Acetone	3,27E-02	1,59E-05	3,24E-04	0,00E+00	2,03E-02	8,17E-04	9,48E-02	3,03E-01
Methyl ethyl ketone/Butanone	7,14E-03	3,46E-06	7,08E-05	0,00E+00	2,67E-03	1,07E-04	6,96E-02	2,23E-01
isopropanol	8,72E-04	4,23E-07	8,65E-06	0,00E+00	0,00E+00	0,00E+00	1,30E-01	4,15E-01
ethyl acetate	7,51E-03	3,64E-06	7,44E-05	0,00E+00	0,00E+00	0,00E+00	2,45E-01	7,84E-01
Other OVOCs	2,32E-01	1,16E-04	2,28E-03	1,43E-04	3,67E-03	3,45E-03	1,74E-01	6,86E-01
Other alkanes	4,14E-02	2,01E-05	4,11E-04	1,43E-04	4,81E-03	1,94E-04	2,31E-02	7,40E-02
Other alkenes	3,22E-01	1,56E-04	3,19E-03	1,79E-03	1,04E-02	4,21E-04	1,50E-02	4,80E-02
Other alkyne	2,86E-02	1,39E-05	2,84E-04	1,43E-04	4,68E-03	1,88E-04	1,50E-02	4,80E-02
Other aromatics	3,81E-02	1,85E-05	3,78E-04	1,43E-04	1,38E-02	5,56E-04	5,36E-02	1,71E-01
Other halocarbons	2,95E-02	1,43E-05	2,92E-04	1,43E-04	4,37E-03	1,76E-04	1,61E-01	5,15E-01

Table S21: OFPs of individual NMVOC species based on integrated emission and source profiles for annual average of 2008-2020 (Unit: Tg-O₃).

Species	transportation	aviation	ships	power	agriculture	waste	residential	industry
Ethane	1,06E-02	5,15E-06	1,05E-04	3,42E-03	2,36E-02	9,52E-04	3,60E-02	1,15E-01
Propane	1,10E-01	5,33E-05	1,09E-03	2,27E-03	6,66E-03	2,68E-04	9,70E-02	3,10E-01
i-Butane	1,49E-01	7,22E-05	1,48E-03	0,00E+00	2,81E-03	1,13E-04	1,28E-01	4,11E-01
n-Butane	1,99E-01	9,64E-05	1,97E-03	5,06E-04	5,98E-03	2,41E-04	1,28E-01	4,10E-01
Cyclopentane	4,36E-02	2,12E-05	4,33E-04	0,00E+00	0,00E+00	0,00E+00	3,09E-02	9,88E-02
i-Pentane	5,75E-01	2,79E-04	5,70E-03	1,12E-03	2,22E-03	8,94E-05	1,10E-01	3,53E-01
n-Pentane	2,41E-01	1,17E-04	2,39E-03	1,27E-03	4,41E-03	1,78E-04	8,67E-02	2,77E-01
Methylcyclopentane	1,41E-01	6,86E-05	1,40E-03	5,45E-04	0,00E+00	0,00E+00	6,87E-02	2,20E-01
Cyclohexane	1,80E-02	8,72E-06	1,78E-04	1,17E-04	0,00E+00	0,00E+00	3,48E-02	1,11E-01
2,2-Dimethylbutane	2,69E-02	1,31E-05	2,67E-04	0,00E+00	3,07E-04	1,24E-05	6,07E-03	1,94E-02
2,3-Dimethylbutane	5,21E-02	2,53E-05	5,17E-04	8,39E-05	3,39E-04	1,37E-05	8,61E-03	2,75E-02
2-Methylpentane	2,51E-01	1,22E-04	2,49E-03	6,38E-04	1,31E-03	5,28E-05	5,63E-02	1,80E-01
3-Methylpentane	2,17E-01	1,05E-04	2,15E-03	2,34E-04	1,65E-03	6,66E-05	5,67E-02	1,81E-01
n-Hexane	6,12E-02	2,97E-05	6,07E-04	8,76E-04	5,15E-03	2,07E-04	1,00E-01	3,21E-01
Methylcyclohexane	3,61E-02	1,75E-05	3,58E-04	1,10E-04	0,00E+00	0,00E+00	3,88E-02	1,24E-01
2,3-Dimethylpentane	2,59E-02	1,26E-05	2,57E-04	3,09E-04	0,00E+00	0,00E+00	1,23E-02	3,92E-02
2,4-Dimethylpentane	2,05E-02	9,94E-06	2,03E-04	0,00E+00	0,00E+00	0,00E+00	3,09E-03	9,89E-03
2-Methylhexane	6,94E-02	3,37E-05	6,89E-04	1,12E-04	8,32E-04	3,35E-05	3,56E-02	1,14E-01
3-Methylhexane	8,21E-02	3,98E-05	8,14E-04	0,00E+00	9,85E-04	3,97E-05	4,24E-02	1,36E-01
n-Heptane	4,43E-02	2,15E-05	4,39E-04	9,10E-04	7,85E-03	3,16E-04	4,65E-02	1,49E-01
2,2,4-Trimethylpentane	5,03E-02	2,44E-05	4,99E-04	0,00E+00	5,51E-05	2,22E-06	4,07E-03	1,30E-02
2,3,4-Trimethylpentane	1,78E-02	8,64E-06	1,77E-04	0,00E+00	0,00E+00	0,00E+00	2,73E-03	8,72E-03
2-Methylheptane	2,04E-02	9,91E-06	2,03E-04	3,63E-04	0,00E+00	0,00E+00	1,47E-02	4,69E-02
3-Methylheptane	1,92E-02	9,29E-06	1,90E-04	1,52E-04	0,00E+00	0,00E+00	1,35E-02	4,31E-02
n-Octane	3,42E-02	1,66E-05	3,39E-04	5,39E-04	1,02E-03	4,12E-05	3,27E-02	1,05E-01
n-Nonane	1,63E-02	7,90E-06	1,61E-04	2,70E-04	0,00E+00	0,00E+00	2,90E-02	9,28E-02
n-Decane	1,55E-02	7,50E-06	1,53E-04	2,65E-04	0,00E+00	0,00E+00	2,43E-02	7,79E-02
n-Un.a.ecane	4,49E-02	2,18E-05	4,45E-04	2,29E-04	0,00E+00	0,00E+00	2,14E-02	6,84E-02
Ethene	1,72E+00	8,33E-04	1,70E-02	8,28E-02	2,26E+00	9,11E-02	6,87E-01	2,20E+00
Propene	9,83E-01	4,77E-04	9,74E-03	7,54E-02	4,55E-01	1,83E-02	2,94E+00	9,39E+00

Table S21 continued from previous page

Species	transportation	aviation	ships	power	agriculture	waste	residential	industry
1,3-butadiene	3,63E-02	1,76E-05	3,60E-04	0,00E+00	4,74E-02	1,91E-03	4,75E-01	1,52E+00
1-Butene	9,65E-01	4,68E-04	9,57E-03	1,04E-02	1,38E-01	5,57E-03	4,10E-01	1,31E+00
cis-2-Butene	1,22E+00	5,93E-04	1,21E-02	1,91E-02	3,86E-02	1,55E-03	1,58E-01	5,07E-01
trans-2-Butene	1,52E+00	7,39E-04	1,51E-02	1,13E-02	7,95E-02	3,20E-03	1,24E-01	3,97E-01
Isoprene	1,03E-01	5,01E-05	1,02E-03	0,00E+00	1,01E-01	4,05E-03	6,15E-02	1,97E-01
1-Pentene	3,10E-01	1,50E-04	3,07E-03	3,74E-03	1,07E-02	4,32E-04	9,70E-02	3,10E-01
cis-2-Pentene	8,24E-01	4,00E-04	8,17E-03	6,73E-04	1,81E-03	7,31E-05	5,51E-02	1,76E-01
trans-2-Pentene	5,32E-01	2,58E-04	5,28E-03	5,33E-04	2,81E-02	1,13E-03	5,12E-02	1,64E-01
1-Hexene	1,20E-01	5,81E-05	1,19E-03	2,14E-03	9,60E-04	3,87E-05	6,38E-02	2,04E-01
Ethylene	2,35E-01	1,14E-04	2,33E-03	4,18E-03	7,61E-02	3,07E-03	1,97E-02	6,30E-02
Benzene	9,88E-02	4,79E-05	9,80E-04	8,51E-03	7,57E-02	3,05E-03	6,21E-02	1,99E-01
Toluene	1,08E+00	5,22E-04	1,07E-02	2,13E-02	1,82E-01	7,35E-03	1,68E+00	5,38E+00
m/p-Xylene	1,00E+00	4,86E-04	9,94E-03	1,26E-02	5,86E-02	2,36E-03	3,24E+00	1,04E+01
Ethylbenzene	2,40E-01	1,16E-04	2,38E-03	1,97E-03	1,89E-02	7,60E-04	9,22E-01	2,95E+00
o-Xylene	4,97E-01	2,41E-04	4,93E-03	4,41E-03	8,95E-02	3,60E-03	1,50E+00	4,78E+00
Styrene	1,07E-01	5,21E-05	1,07E-03	6,24E-05	1,29E-02	5,21E-04	4,96E-01	1,59E+00
1,2,3-Trimethylbenzene	4,67E-01	2,26E-04	4,63E-03	1,90E-03	3,40E-02	1,37E-03	5,24E-01	1,68E+00
1,2,4-Trimethylbenzene	7,40E-01	3,59E-04	7,34E-03	2,37E-03	2,56E-02	1,03E-03	5,71E-01	1,83E+00
1,3,5-Trimethylbenzene	1,94E-01	9,43E-05	1,93E-03	1,10E-03	1,44E-02	5,80E-04	4,14E-01	1,32E+00
i-Propylbenzene	5,19E-02	2,52E-05	5,15E-04	3,63E-05	4,40E-04	1,77E-05	4,83E-02	1,54E-01
m-Ethyltoluene	1,69E-01	8,18E-05	1,67E-03	1,15E-03	1,03E-02	4,16E-04	4,09E-01	1,31E+00
n-Propylbenzene	3,44E-01	1,67E-04	3,41E-03	2,56E-04	3,88E-03	1,56E-04	1,10E-01	3,52E-01
o-Ethyltoluene	2,48E-01	1,20E-04	2,46E-03	5,54E-04	1,92E-03	7,73E-05	1,44E-01	4,60E-01
p-Ethyltoluene	1,19E-01	5,76E-05	1,18E-03	5,15E-04	3,84E-03	1,55E-04	1,46E-01	4,68E-01
m-Diethylbenzene	2,26E-01	1,10E-04	2,24E-03	4,61E-04	0,00E+00	0,00E+00	5,49E-02	1,76E-01
p-Diethylbenzene	9,31E-02	4,52E-05	9,23E-04	7,98E-04	0,00E+00	0,00E+00	7,42E-02	2,37E-01
tetrachloromethane	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
Chloroform	8,28E-06	4,02E-09	8,21E-08	0,00E+00	0,00E+00	0,00E+00	4,84E-04	1,55E-03
Dichloromethane	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
Chloromethane	0,00E+00	0,00E+00	0,00E+00	0,00E+00	3,94E-04	1,59E-05	1,23E-03	3,93E-03
Tetrachloroethylene	9,20E-07	4,46E-10	9,13E-09	0,00E+00	0,00E+00	0,00E+00	1,55E-04	4,96E-04

Table S21 continued from previous page

Species	transportation	aviation	ships	power	agriculture	waste	residential	industry
Vinyl chloride	9,20E-07	4,46E-10	9,13E-09	0,00E+00	0,00E+00	0,00E+00	7,73E-03	2,47E-02
Formaldehyde	1,42E+00	6,86E-04	1,40E-02	0,00E+00	1,50E+00	6,04E-02	0,00E+00	0,00E+00
Acetaldehyde	3,46E-01	1,68E-04	3,44E-03	0,00E+00	6,33E-01	2,55E-02	0,00E+00	0,00E+00
acrolein	1,09E-01	5,30E-05	1,08E-03	0,00E+00	7,81E-02	3,15E-03	0,00E+00	0,00E+00
Methanol	2,68E-01	0,00E+00	5,43E-04	0,00E+00	3,03E+00	0,00E+00	1,47E+00	1,99E-01
Ethanol	3,75E-04	0,00E+00	5,19E-03	0,00E+00	2,98E+01	0,00E+00	1,96E+00	5,47E+00
Propionaldehyde/Propanal	6,16E-02	2,99E-05	6,11E-04	0,00E+00	7,87E-02	3,17E-03	0,00E+00	0,00E+00
Butyraldehyde/n-Butanal	1,29E-01	6,24E-05	1,28E-03	0,00E+00	5,71E-02	2,30E-03	0,00E+00	0,00E+00
Valeraldehyde/n-Pentanal	5,01E-02	2,43E-05	4,97E-04	0,00E+00	7,92E-02	3,19E-03	0,00E+00	0,00E+00
Isovaleraldehyde	3,30E-02	1,60E-05	3,28E-04	0,00E+00	2,60E-02	1,05E-03	0,00E+00	0,00E+00
Benzaldehyde	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
Hexanaldehyde/n-Hexanal	7,96E-02	3,86E-05	7,90E-04	0,00E+00	1,12E-01	4,53E-03	0,00E+00	0,00E+00
Acetone	1,18E-02	5,71E-06	1,17E-04	0,00E+00	7,30E-03	2,94E-04	3,41E-02	1,09E-01
Methyl ethyl ketone/Butanone	2,77E-02	1,34E-05	2,75E-04	0,00E+00	1,03E-02	4,17E-04	2,70E-01	8,64E-01
isopropanol	5,32E-04	2,58E-07	5,27E-06	0,00E+00	0,00E+00	0,00E+00	7,91E-02	2,53E-01
ethyl acetate	5,40E-04	2,62E-07	5,36E-06	0,00E+00	0,00E+00	0,00E+00	1,77E-02	5,65E-02
Other OVOCs	1,26E+00	6,13E-04	1,24E-02	0,00E+00	0,00E+00	1,98E-02	1,29E+00	4,27E+00
Other alkanes	1,66E-01	8,04E-05	1,64E-03	5,72E-04	1,92E-02	7,75E-04	9,25E-02	2,96E-01
Other alkenes	1,17E+00	5,69E-04	1,16E-02	6,57E-03	2,71E-02	1,09E-03	0,00E+00	0,00E+00
Other alkyne	0,00E+00	0,00E+00	0,00E+00	0,00E+00	4,02E-03	1,62E-04	0,00E+00	0,00E+00
Other aromatics	3,80E-02	1,84E-05	3,77E-04	0,00E+00	4,06E-02	1,63E-03	1,54E-01	4,94E-01
Other halocarbons	3,58E-03	1,74E-06	3,55E-05	0,00E+00	2,80E-03	1,13E-04	5,84E-01	1,87E+00

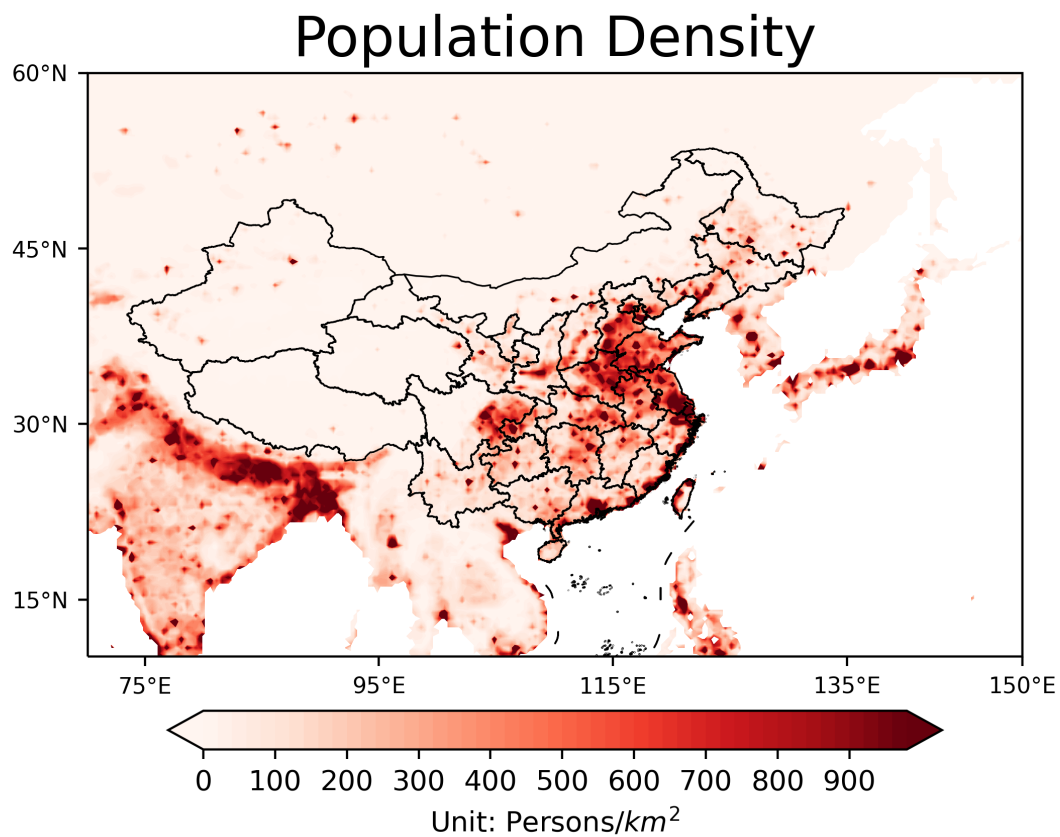
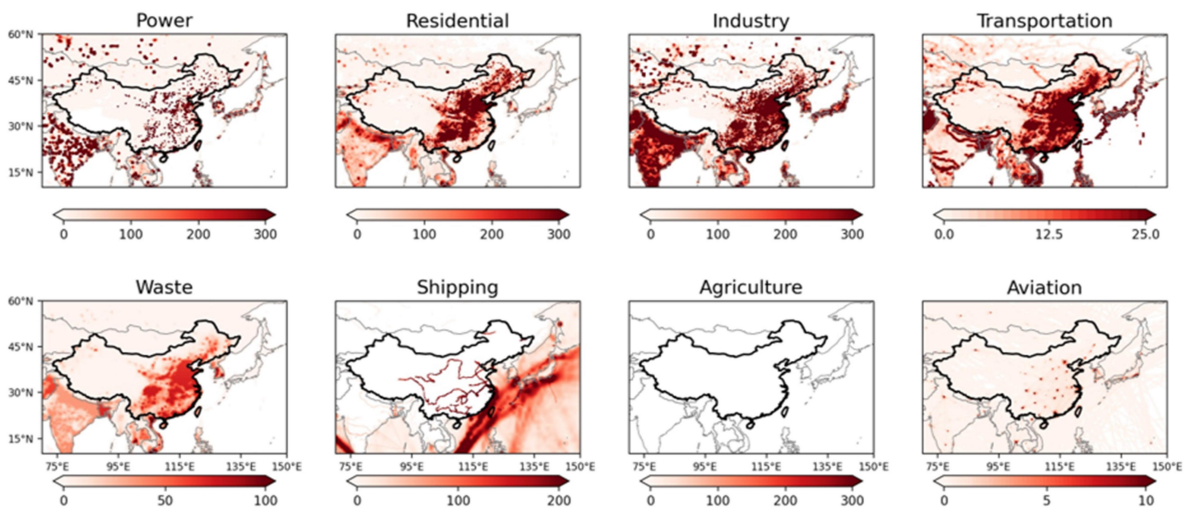
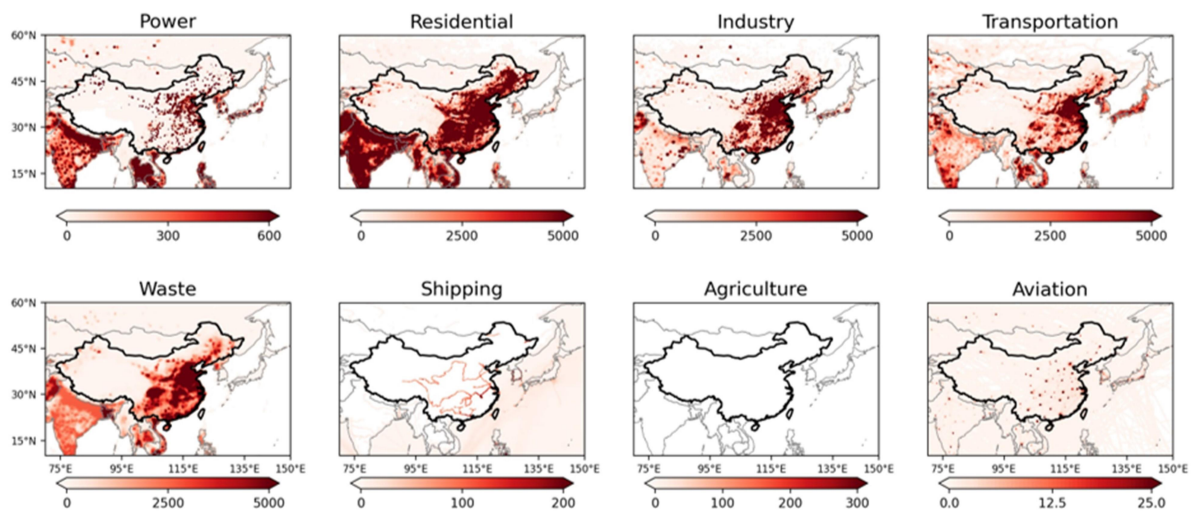


Figure S18. Spatial distribution of population in Eastern Asia (persons km^{-2}) in 2020. The data product is Gridded Population of the World, Version 4 (GPWv4, <https://sedac.ciesin.columbia.edu/data/collection/gpw-v4/documentation>, last accessed: June, 2024). The spatial resolution is 30 km^{-2} .

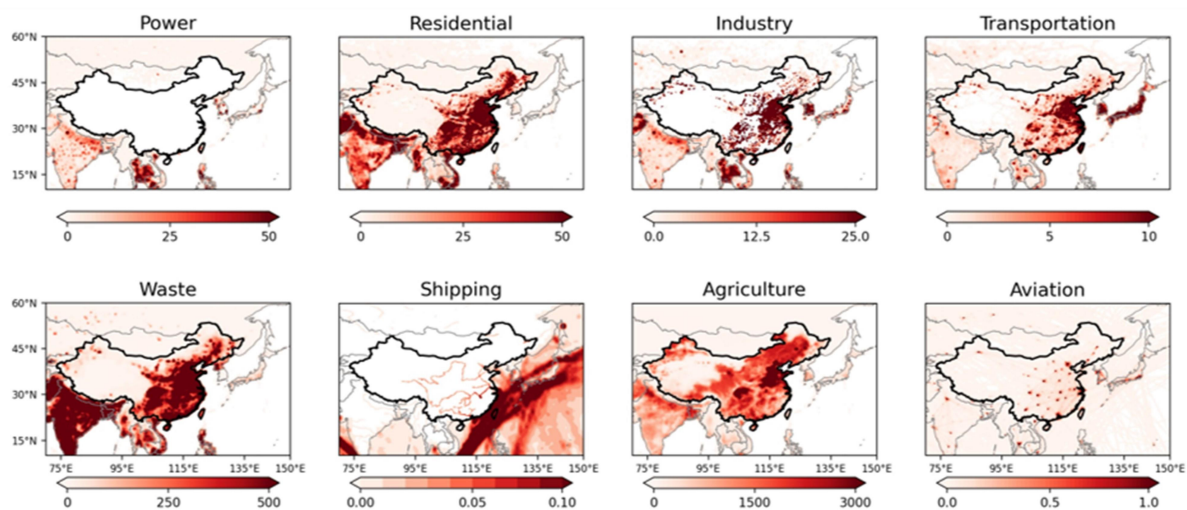
(a) SO₂ in 2017 (ton grid⁻¹ yr⁻¹)



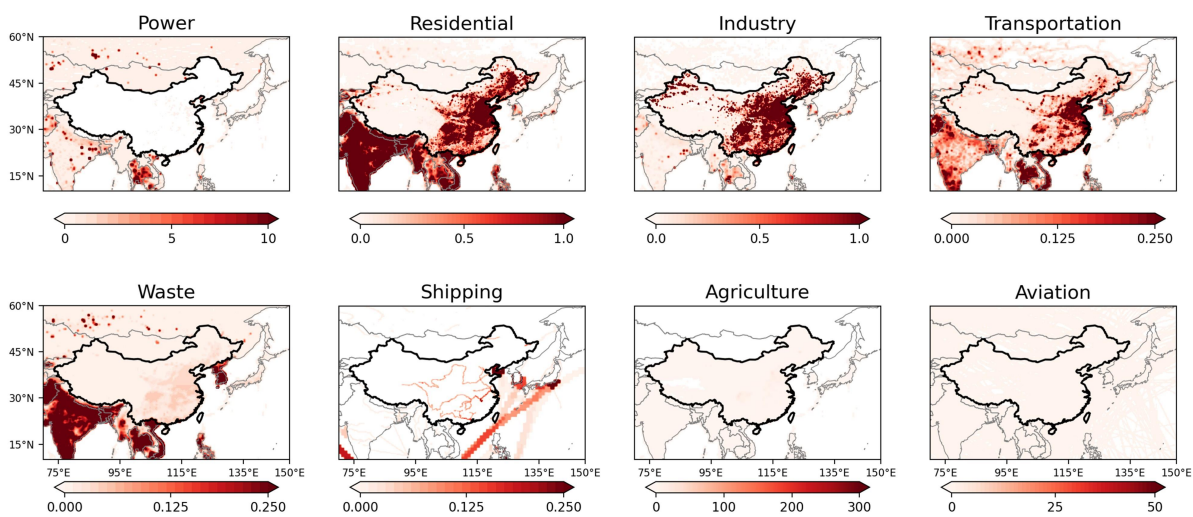
(b) CO in 2017 (ton grid⁻¹ yr⁻¹)



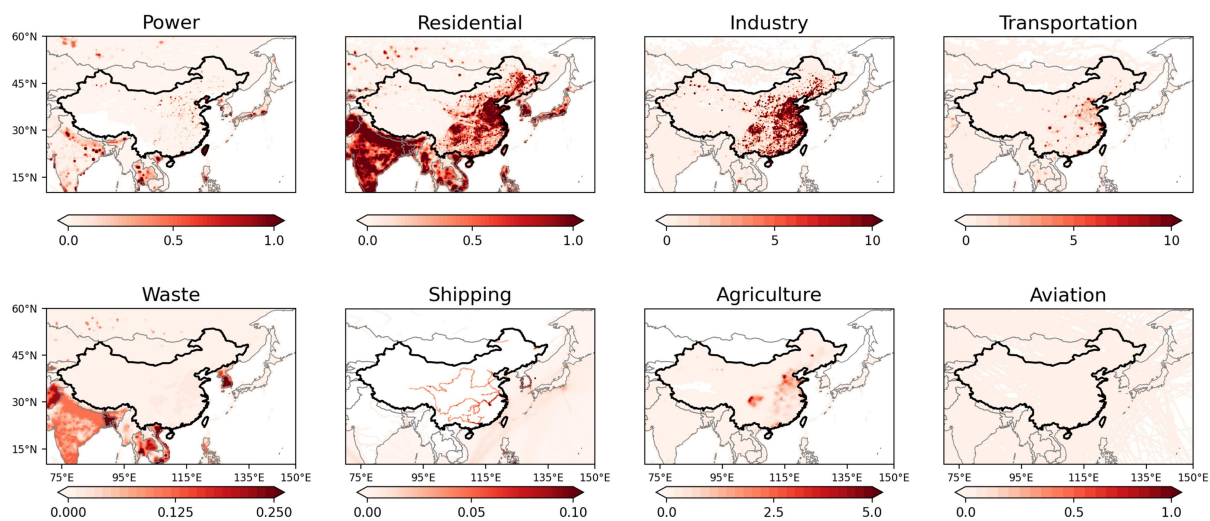
(c) NH_3 in 2017 ($\text{ton grid}^{-1} \text{ yr}^{-1}$)



(b) C_2H_6 in 2017 ($\text{ton grid}^{-1} \text{ yr}^{-1}$)



(e) Toluene in 2017 (ton grid⁻¹ yr⁻¹)



(f) C₂H₄ in 2017 (ton grid⁻¹ yr⁻¹)

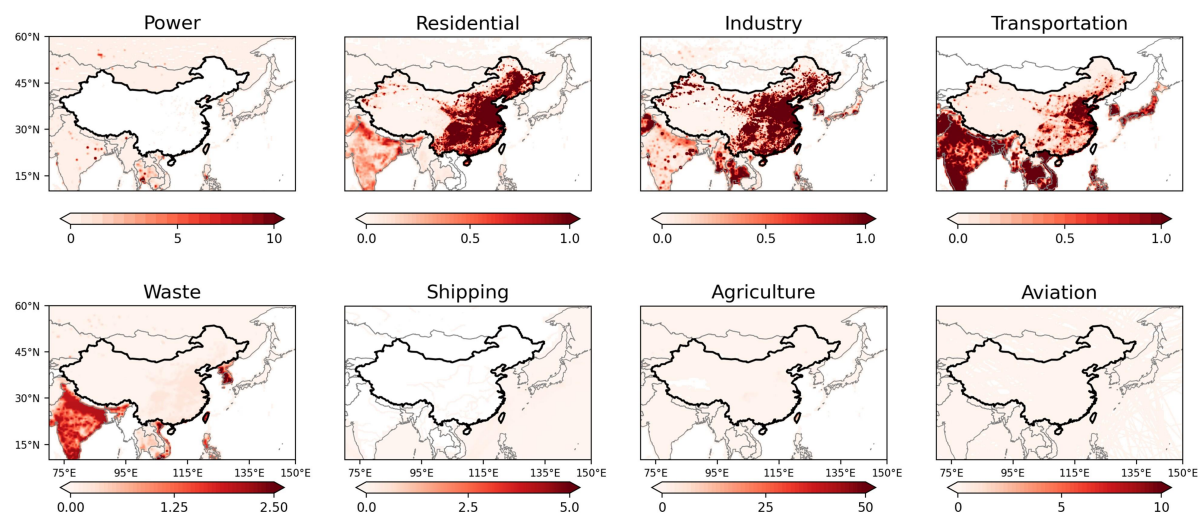


Figure S19. CINEI spatial distribution of SO₂, CO, NH₃, C₂H₆, Toluene, and C₂H₄ emission (ton grid⁻¹ year⁻¹) in 2017.

NO_x in January 2017

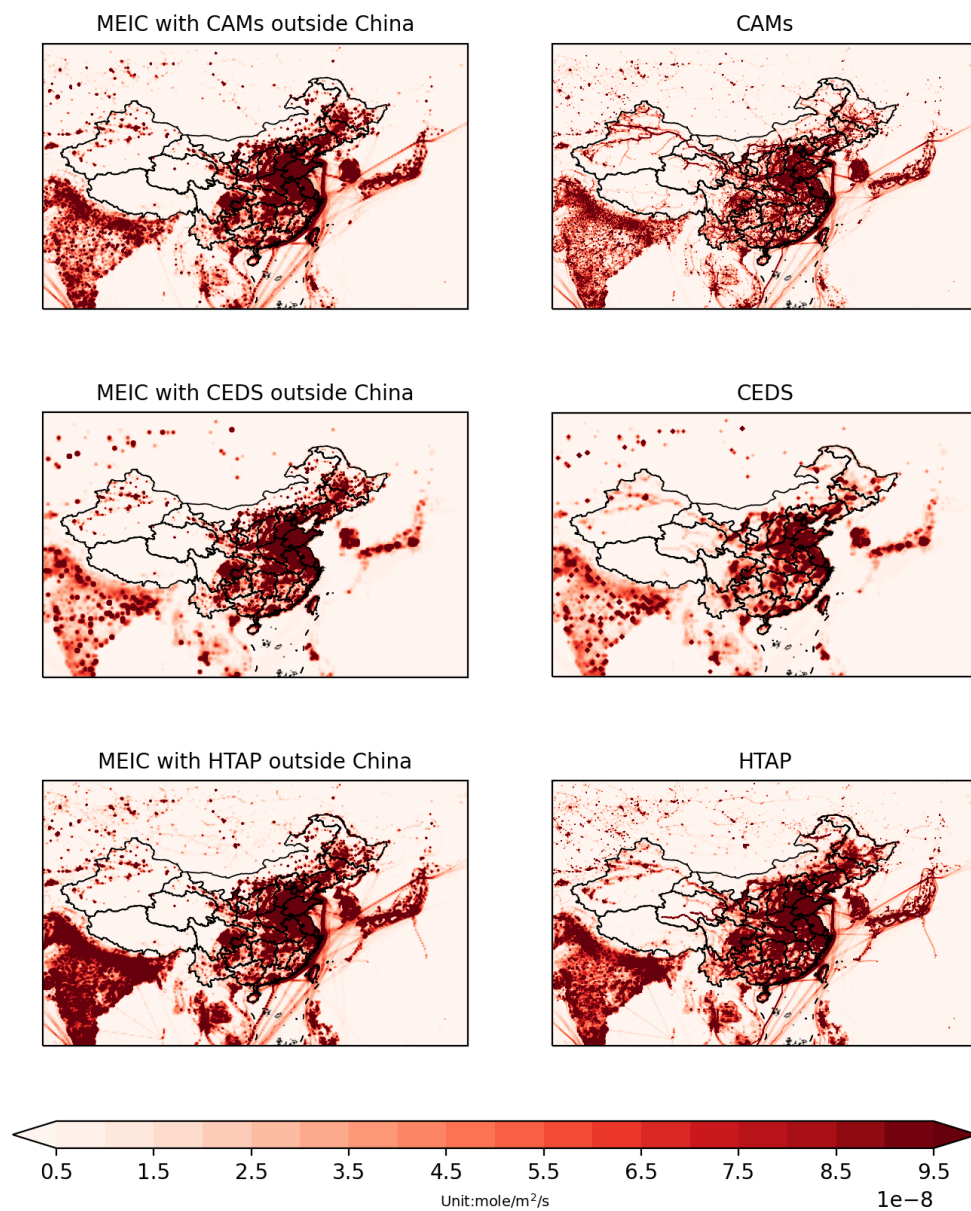


Figure S20. HMEIs and global emission inventories' spatial distribution of NO_x (NO₂) emissions ($\text{mol m}^{-2} \text{s}^{-1}$) in January, 2017.

C₂H₄ in January 2017

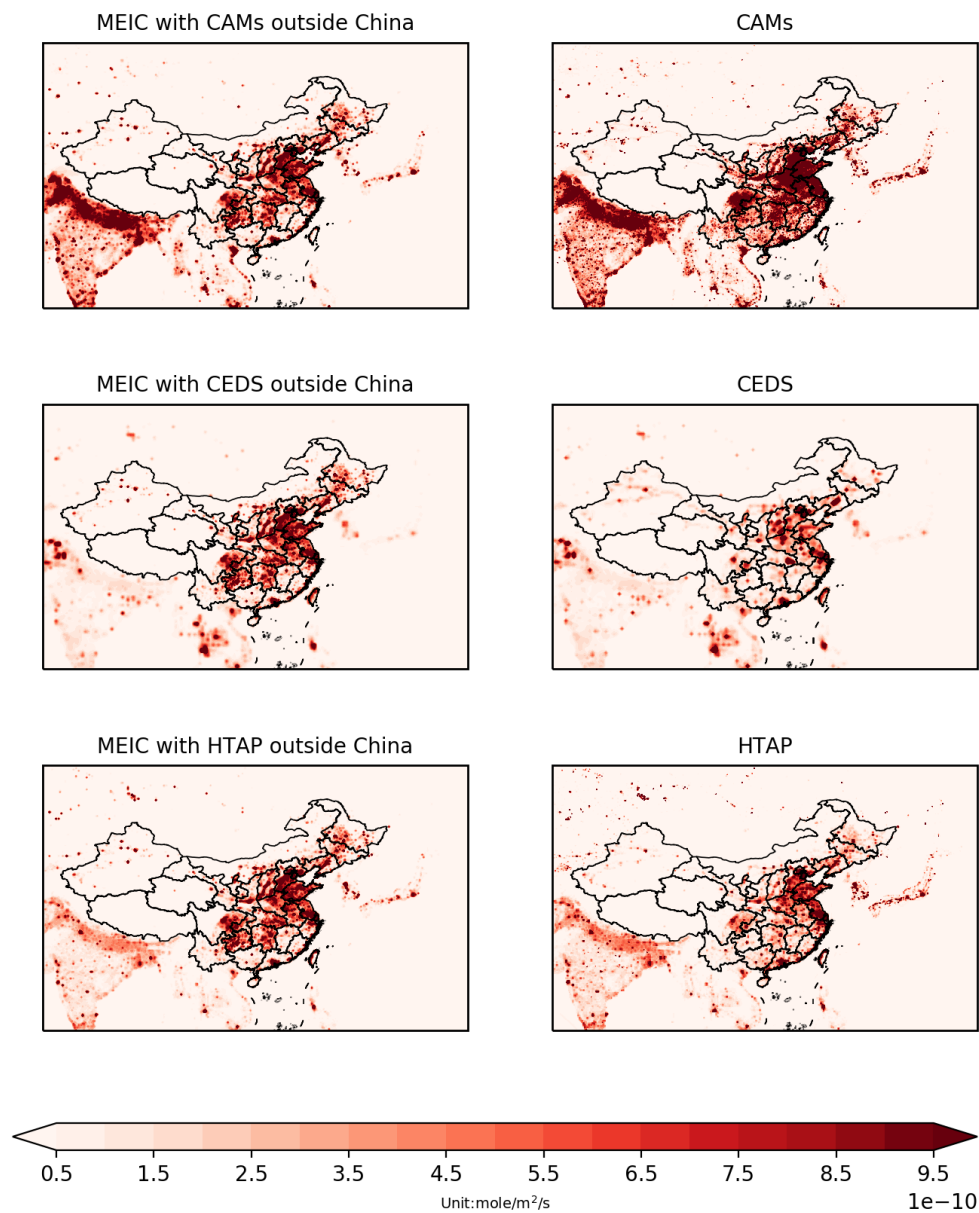


Figure S21. HMEIs and global emission inventories' spatial distribution of C₂H₄ emissions (mol m⁻² s⁻¹) in January, 2017.

NO_x in July 2017

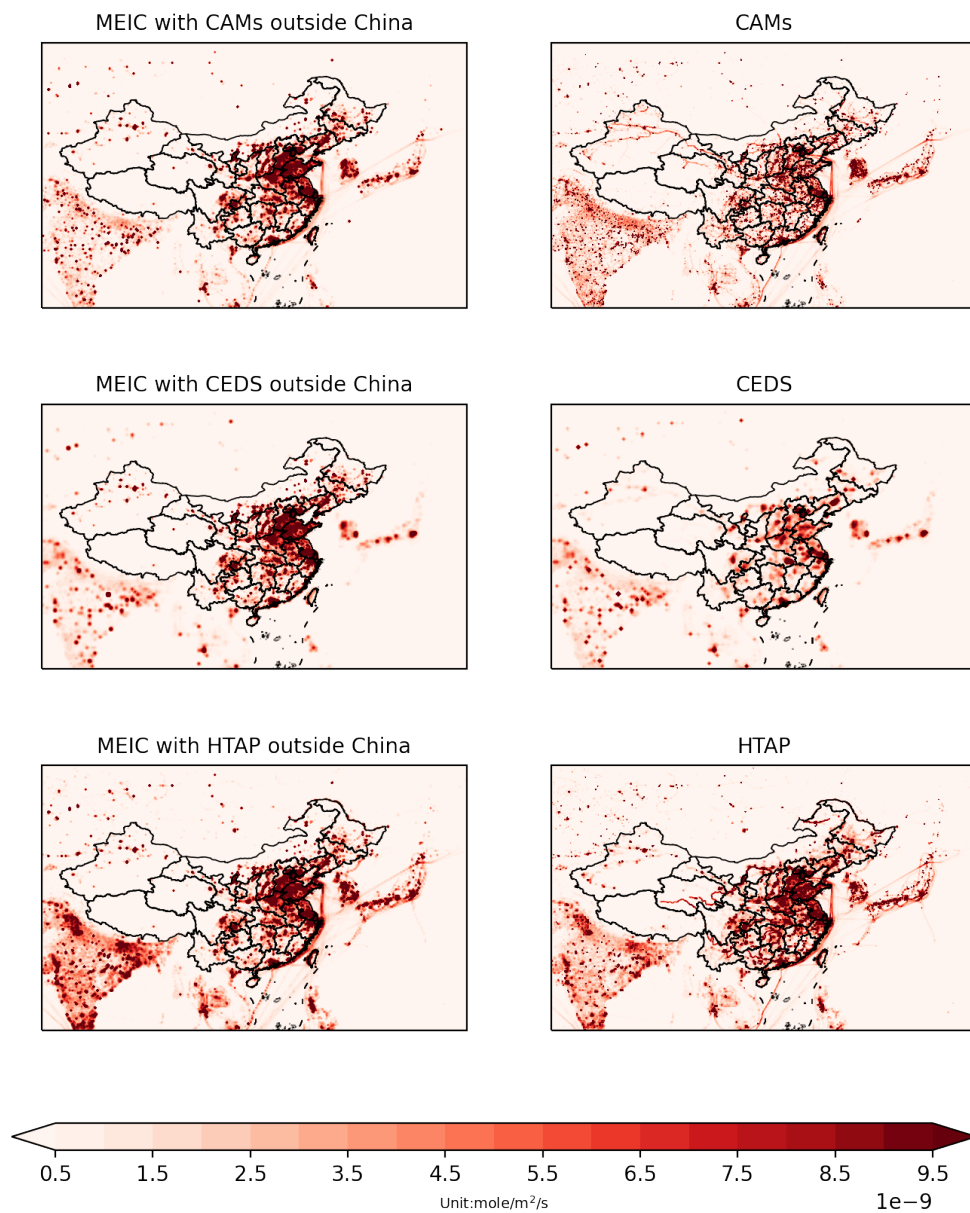


Figure S22. HMEIs and global emission inventories' spatial distribution of NO_x (NO₂) emissions (mol m⁻² s⁻¹) in July, 2017.

C₂H₄ in July 2017

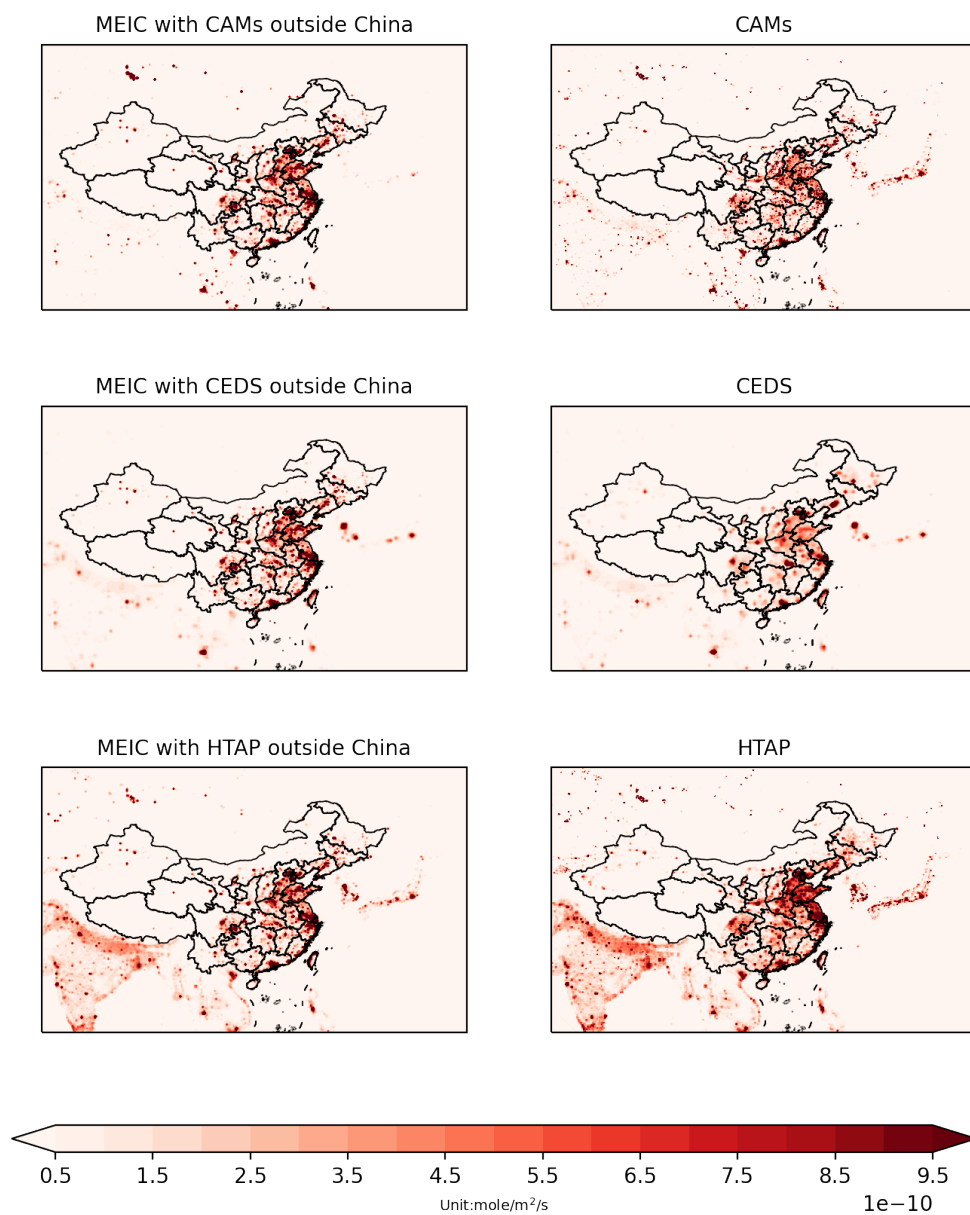


Figure S23. HMEIs and global emission inventories' spatial distribution of C₂H₄ emissions (mol m⁻² s⁻¹) in July, 2017.

In addition to emissions within mainland China, emissions from surrounding regions are derived from different global emission inventories, and the emitted pollutants might impact air quality in local and remote areas via wind transport. This raises concerns about the accuracy of regional emissions around targeted region. To accurately represent scenarios in the surrounding region, careful selection and validation of global inventories is important. In this section, we utilize three harmonized emission
290 inventories (HM_CEDS, HM_CAMs, and HM_HTAP), all maintaining the same emission amounts from the national emission inventory (MEIC) in mainland China but varying emissions from the global CEDS, CAMs, and HTAP emission inventories, respectively. Modeling mixing ratios based on harmonized emission inventories located on eastern coastal cities (Figure S25) will be compared with observations on diurnal and spatial scales. We investigate horizontal wind directions at ground level in two seasons: prevailing southeasterly winds (wind direction 160° , wind speed 3.6 m s^{-1} in the summer transport pollutants
295 from the East Sea and Korea within the area of interest, while prevailing northwesterly winds in the winter have little effect on regional transport. Therefore, winter conditions will not be discussed in this section. We select 11 coastal cities around the East sea, with high exposure to external emissions. Validations of meteorological fields (including temperature at 2m, wind speed and wind direction at 10 m) are provided in Table S23 and Table S24.

For spatial distribution (Figure S25), the prevailing southeasterly winds in summer result in impactful emissions from the
300 East China Sea, Bohai Sea, and Korea, influencing air quality in the North China Plain (NCP). Concerning the spatial mean for the entire region, modeling ozone mixing ratios of HM_HTAP and HM_CAMs are lower than those of HM_CEDS in both surrounding regions and mainland China, with -2 ppbv and -6.3 ppbv respectively. Conversely, NO_2 is higher by 0.95 ppbv and 0.07 ppbv. CO shows no significant change for average on entire region of interest. Consequently, our harmonized emission inventories, which adjusts emissions outside eastern China while preserving the NCP, serves as an illustrative case
305 for understanding local and regional pollution dynamics.

Figure S24 shows the comparisons between the modeling results of three harmonized emission inventories in the two months and the observations. We found that the mixing ratios of three cases in each season do not show significant variation for averages of the whole domain, but have a notable deviation in coastal cities where there is exposure to external emissions from global emission inventories. In winter, ozone mixing ratios of three emission inventories are overestimated for whole regions
310 (20-40%) and coastal cities (2-25%). NO_x mixing ratios are overestimated by 40% for whole regions, but underestimated by -10-20% for coastal cities. The harmonized CEDS emission inventory are slightly closer to the observed CO mixing ratios by 6.3% (coastal cities) and -20% (whole area). In summer, O_3 and NO_2 mixing ratios are generally overpredicted by all emission inventories, and HM_CAMs and HM_HTAP emission inventories show the largest bias for NO_2 mixing ratios, by 159% and 296% respectively. In addition, the CO simulation in coastal cities is better than the results for the whole domain, which may
315 be due to waste emissions in Korea and Japan. After above comparing the modeling results with observations, we favor the global CEDS emission inventory for providing emissions data around mainland China.

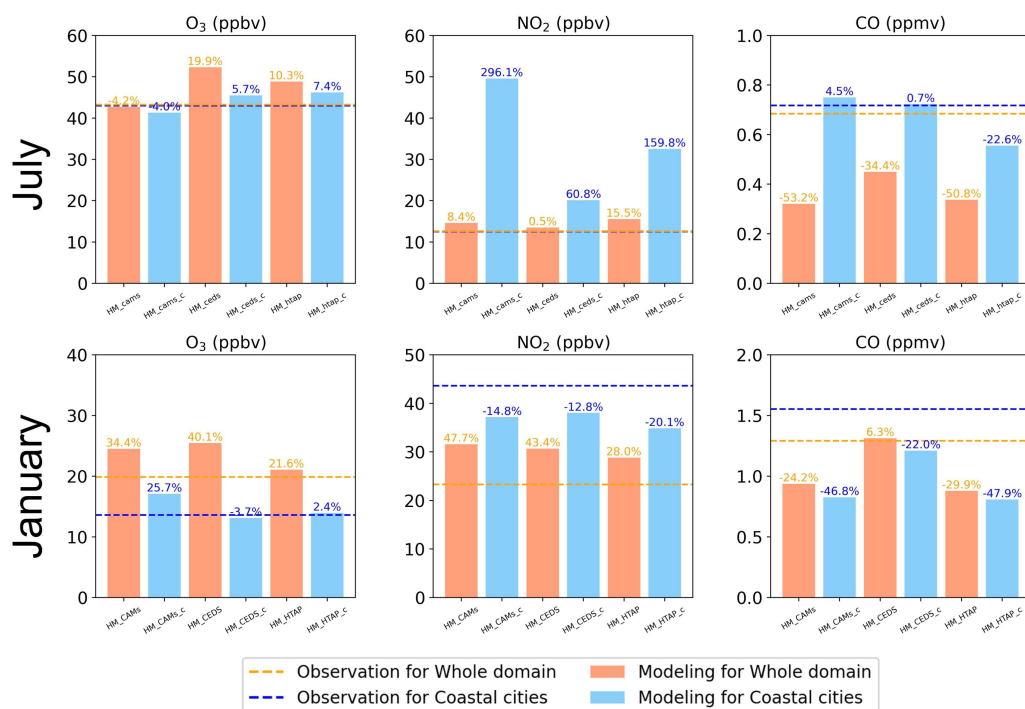


Figure S24. Validation of modeling mixing ratios for O₃ (ppbv), NO₂ (ppbv) and CO (ppmv) based on harmonised emission inventories (HM_CEDS, HM_CAMs and HM_HTAP) against observations in July and January 2017. The ticks on axes such as 'HM_CEDS' represent modelled values for averaged all grids, including observed sites for the whole domain. Orange horizontal lines represent observed averages for whole domain, and blue lines represent observed averages for coastal cities affected by emissions outside mainland China. The ticks on axes such as "HM_CEDS_c" represent model values for averaged all grids including observed sites for coastal cities. The coastal cities are shown in Fig. S25.

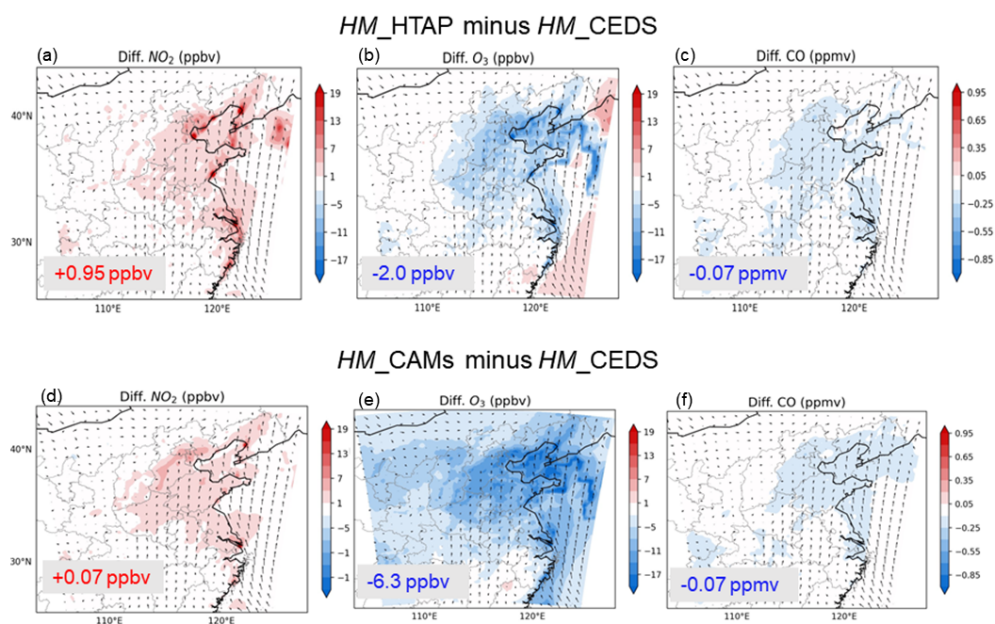


Figure S25. Differences of ozone, NO₂, and CO mixing ratios across harmonized emission inventories on spatial scale in July 2017.

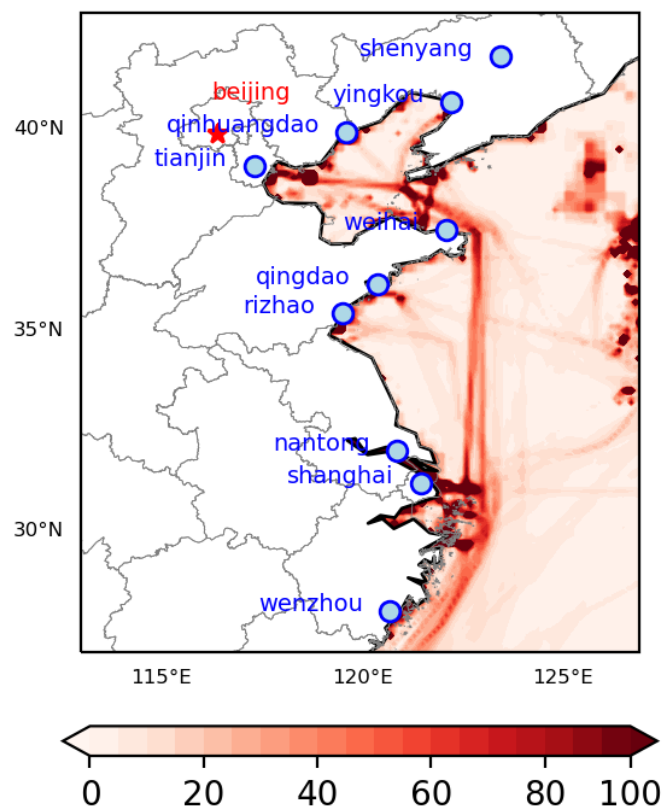


Figure S26. Spatial distribution of coastal cities that are exposed to emissions from different global emission inventories. These cities are selected for validations of harmonized emission inventories.

S13 Analysis of Modeling Bias

Summer Evaluation

Figure S27 show statistical metrics of evaluation for O₃, CO, and NO₂ in summer. In general, comparison of evaluation across different emission inventories demonstrates that integrated and harmonized emission inventories significantly outperform global emission inventories regarding ozone and NO₂. Modeling CO mixing ratios in all cases are underestimated.

Ozone concentration in summer is higher than in winter, and the CINEI case slightly overestimates ozone with NMB of 0.11 and MNB of 0.05. Indicators of MNAE and MAE for CINEI add to better performance: 0.17 and 7.18 for ozone respectively, and 0.34 and 4.01 for NO₂ respectively. Comparing with harmonized EI, CINEI improved the ozone performance and reduced the bias by 10% NMB, 9% MNB, 7% MNAE, and 5% MFB. Both CINEI and Harmonized emission inventory present similar performance for NO₂ mixing ratios, with 0.05 and 0.07 NMB, -0.25 and -0.18 MNB, 0.34 and 0.33 MNAE, 4.01 and 3.9 MAE respectively. Inclusion of agricultural and shipping NO_x emission in integrated emission inventory has not impacted modeling NO₂ mixing ratio significantly, but ozone using integrated emission inventory got closer to observation. We need to take changes of NMVOC emissions and their OFPs into account.

Compared with global emission inventories, the CAM emission inventory underestimated ozone by -0.28 NMB and -0.57 MNB. This is mainly due to a large reduction of NMVOC emission in CAMs inventory. CINEI improved the performance and reduced bias by 16% NMB, 50% MNB, 15% MNAE, and 16% MFB.

HTAP case overestimated ozone with 0.11 NMB, 0.04 MNB, and 0.07 MFB. For absolute bias, the HTAP case has a relatively higher bias than other cases, with 0.17 MNAE and 10.9 MAE. This suggests the modeling errors are distributed on the higher inter-quantile part.

CEDS case shows good agreement with observational ozone, with 0.05 NMB, 0.03 MNB, 0.14 MNAE, and 0.04 MFB. CEDS shows better agreement with observation in global emission inventories.

Furthermore, modelling performance based on CINEI in July 2017 is superior to that based on MIXv2, as illustrated in Figure S29 and Table S22. All MIX elements show underestimation: NO₂ by 7 ppbv (-54%), CO by 0.5 ppmv (-85%) and O₃ by 14 ppbv (-34%). The underestimations are likely due to (1) the missing sectors like aviation and agriculture lead to reduced NO_x and CO emission. (2) the emission transported from region around China and from ocean. China's emission of CINEI is incorporated into CEDS inventory, while MIX inventory is using CAPSS for Korea and MOEJ for Japan, (3) MIX inventory provides NMVOCs species as high-lumped species, which might lead to missing reactivity of NMVOCs species in WRF-Chem model. Due to the limitations of the supercomputing resources available, we did not conduct the experiments in January.

Winter Evaluation

Figure S28 shows statistical metrics of evaluation for O₃, CO, and NO₂ in winter. In general, comparison of evaluation across different emission inventories demonstrates that integrated and harmonized emission inventories have relatively lower bias compared with global emission inventories.

Ozone concentration in winter is lower than in summer, so that metrics, such as NMB, MNB of ozone are larger than ones in summer in all cases. Modeling ozone concentration using integrated and harmonized emission inventories shows no evident

changes, with 0.24 and 0.21 NMB, 0.24 and 0.22 MNB, 0.43 and 0.45 MNAE, 0.31 and 0.28 MFB respectively. CO mixing ratios in the two cases are still underestimated by -0.38 NMB, -0.36 MNB, and 0.93 MFB.

355 Ozone formation in winter is under control of NO_x -saturated photochemistry regime. With fewer available radicals in the winter, ozone shows reduction with NO_x increasing, due to termination rate of NO_x -OH being faster than OH-OH reaction. Ozone concentration tends to be decreased with NO_x increase, and is not sensitive to NMVOCs emission changes during winter.

HTAP case underestimated ozone with -1.1 NMB, -1.65 MNB, and -0.78 MFB. Together with 0.17 MNAE and 10.57 MAE, the HTAP case has extremely lower values, which means modeling errors are distributed on the lower inter-quantile part.
360 Regarding global emission inventories, CAMs emission inventory underestimated ozone by -0.43 NMB, and -0.52 MNB, due to higher NO_x emission. CINEI improved the performance and reduced bias by 19% NMB, 28% MNB, and 13% MNAE.

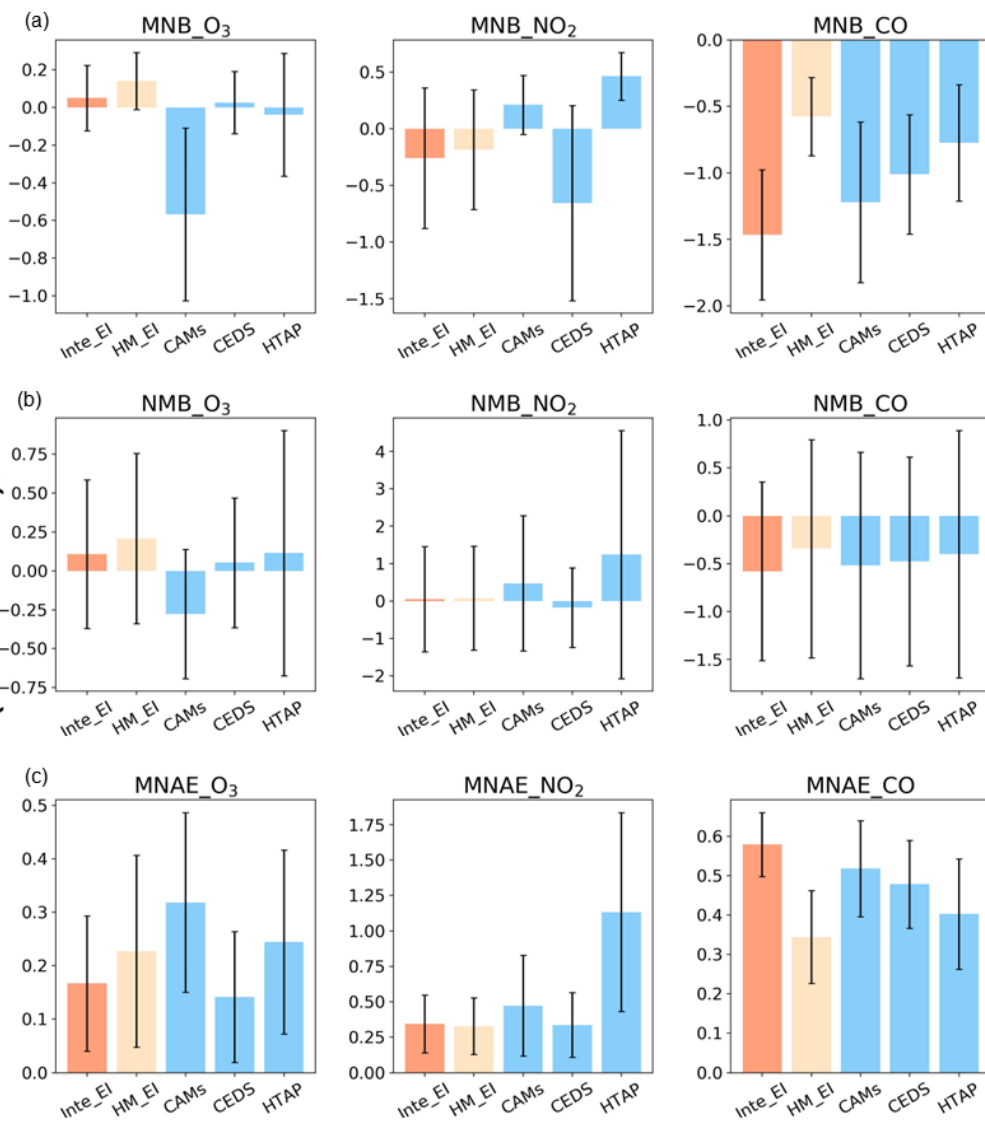
Comparison with literature

We also refer to the modeling performance for air pollutants, emission inventories, and meteorological conditions, evaluated by previous literature. Hu et al. (2017) simulated air pollutants using WRF-CMAQ and four emission inventories (MEIC, EDGAR, and REAS2) in 2013, and the annual O_3 bias ranges from -0.04 to 0.2 for MFB, and 0.28 to 0.33 for mean normalized errors (MNE). CO is also underestimated by all cases, with -0.72 to -1.12 for MFB, and 0.59 to 0.73 for MNE. NO_2 ranges from 0.81 to 1.07 for MFE, and 0.66 to 0.67 for MNE. The ensemble annual daily maximum 1h O_3 (O_3 -1h) concentrations are also improved, with a MNB of 0.03 and MNE of 0.14, compared to an MNB of 0.06–0.19 and MNE of 0.16–0.22 for the individual predictions.
365

370 Saikawa et al. (2017) used WRF-Chem to assess the difference in O_3 simulation for January and July 2008 with REAS v2.1, EDGAR v4.2, and MEIC. For January, a slight difference was found between REAS and EDGAR simulations, while the O_3 levels simulated with MEIC were 31% and 25% lower than those with EDGAR for central and eastern China, respectively. For July, a maximum difference of 8.5 ppb was simulated between the three inventories, and the application of REAS resulted in a larger high- O_3 -polluted area due to the high VOCs emissions. Given this bias, Zheng et al. (2021) expanded the point source database for China and developed a 1-km resolution emission inventory.

Zhai et al. (2024) reported the criteria for $\text{PM}_{2.5}$ simulation in the CTM model based on literature investigation, and the NMB for total $\text{PM}_{2.5}$ should be within 10% and 20%, while the NME should be within 35% and 45%, respectively. We evaluated the model performance of O_3 since 2010, with different models and simulations and analyzed the main factors influencing the simulation. The R between simulation and observation were larger than 0.5, and the NMB were within $\pm 30\%$ for nearly 80% of the cases collected from air quality modeling studies. The Goddard Earth Observing System with Chemistry model (GEOS-Chem) and Comprehensive Air Quality Model with extensions (CAMx) commonly overestimated surface O_3 concentration in China, indicated by the positive medians of NMBs at 14% and 7%, respectively (Jin et al., 2011). Zhong et al. (2016) found comparable O_3 simulation performances with the two inventories for July 2007, indicated by the R around 0.8 and NMB around 19% between the simulation and observation.
380

Jul (Summer), 2017



Statistical metrics (MNB, NMB, and MNAE) for evaluating O₃, CO, and NO₂ mixing ratios against observation in July 2017.

Jul (Summer), 2017

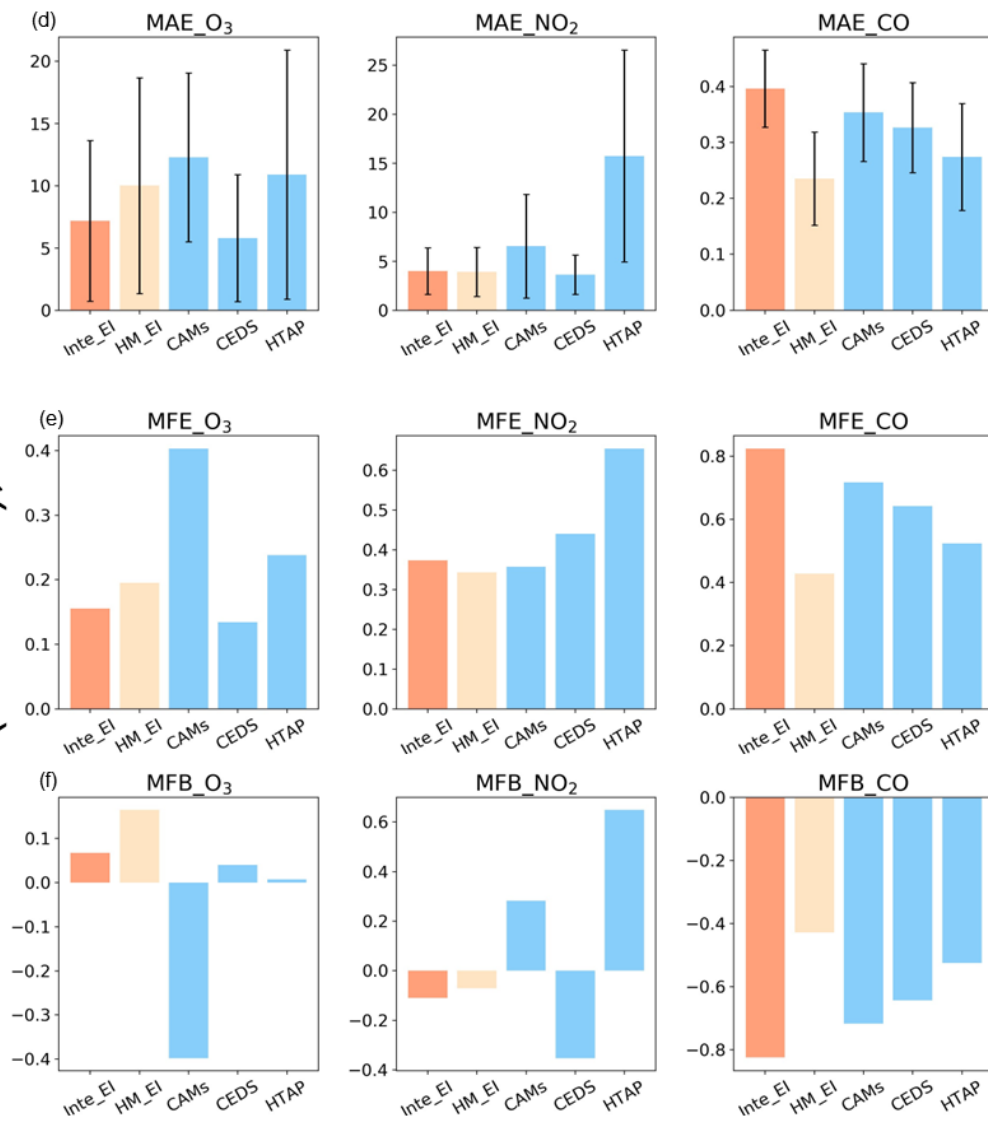
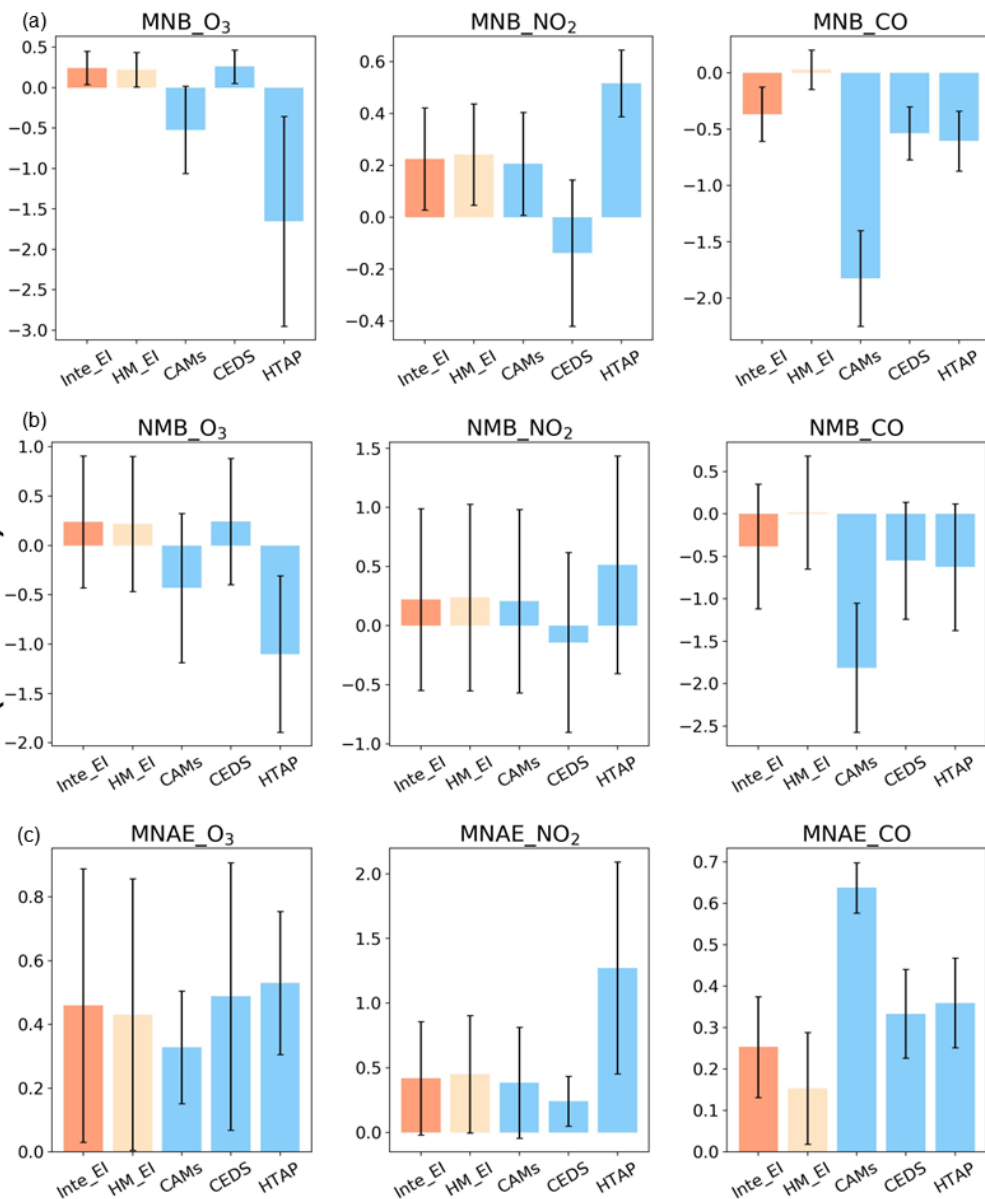


Figure S27. Statistical metrics (MAE, MFE, and MFB) for evaluating O₃, CO, and NO₂ mixing ratios against observation in July 2017.

Jan (Winter), 2017



Statistical metrics (MNB, NMB, and MNAE) for evaluating O₃, CO, and NO₂ mixing ratios against observation in January 2017.

Jan (Winter), 2017

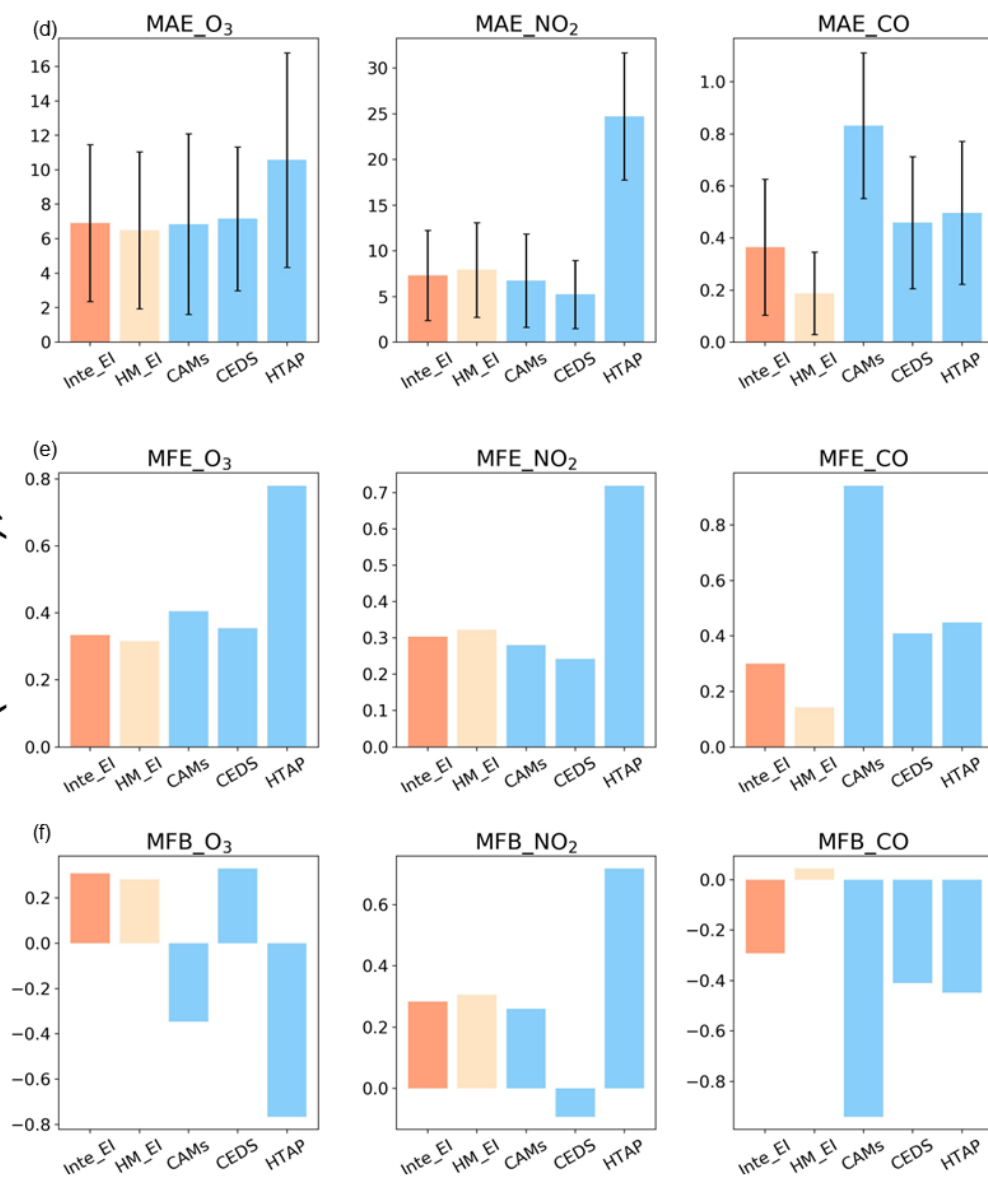


Figure S28. Statistical metrics (MAE, MFE, and MFB) for evaluating O₃, CO, and NO₂ mixing ratios against observation in January 2017.

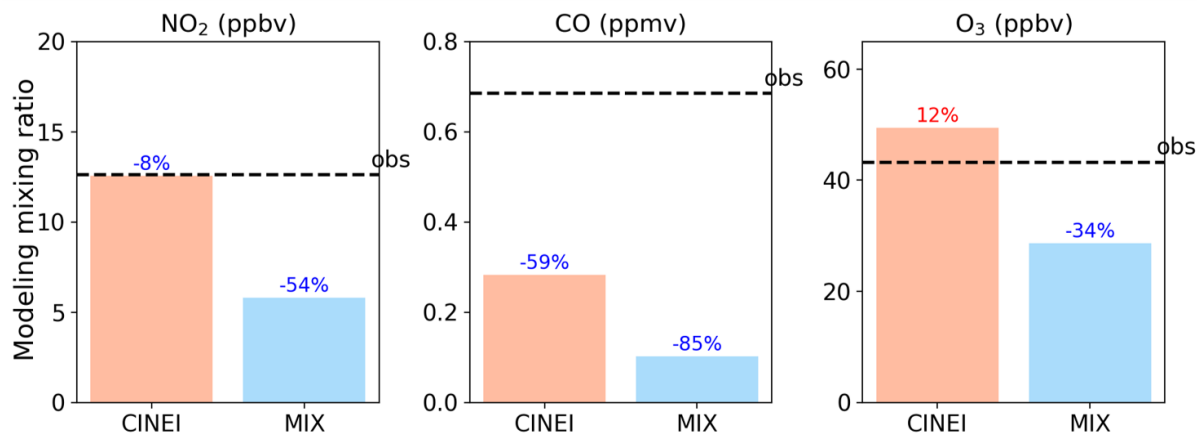


Figure S29. WRF-Chem simulated mixing ratios of O₃, NO₂, and CO for July 2017 (summer) and within the modeling domain using CINEI (in orange) and MIX (in blue). Individual columns show simulated mean mixing ratios in the model domain for each emission inventory used. The dashed blue lines show average observed mixing ratios calculated using the stations within the specified domain. The numbers on the columns are Normalized mean bias (NMB). Blue (red) number indicates underestimated (overestimated).

385 Furthermore, modeling performance based on CINEI in July 2017 outperforms that based on MIXv2, as illustrated in Figure S29 and Table S22. The MIXv2-based runs substantially underestimated all three pollutants: NO₂ by 7 ppbv (-54%), CO by 0.5 ppmv (-85%), and O₃ by 14 ppbv (-34%). These underestimations likely result from (1) missing emission sectors such as aviation and agriculture, leading to lower NO₂ and CO emissions and (2) incomplete accounting for transported emissions from surrounding regions and the ocean. CINEI integrates China's emissions within the CEDS inventory, while MIXv2 uses
390 other regional inventories (CAPSS for Korea and MOEJ for Japan). Additionally, MIXv2 inventory provides NMVOCs species as high-lumped species, which might lead to missing reactivity of NMVOCs species in WRF-Chem model.

Table S22. CINEI and MIX Model Performance Metrics for O₃, NO₂, and CO

Metric	O3 (ppbv)		CO (ppmv)		NO2 (ppbv)	
	MIX	CINEI	MIX	CINEI	MIX	CINEI
Observed	43.24	43.24	0.68	0.68	12.61	12.61
Model	28.68	49.46	0.10	0.28	5.79	12.54
NMB (%)	-34	12	-85	-59	-54	-8
MFB (%)	-42	10	-149	-84	-88	-17
MNAE (%)	34	18	85	59	58	34
R	0.95	0.95	0.28	0.50	0.85	0.85

Table S23. Validation of meteorological conditions using observational data for coastal sites in July 2017.

Parameter	Temp (Kelvins)	Wind speed (m s ⁻¹)	Wind direction (°)
Observed average	303.7	3.6	169.7
Model average	300.7	3.6	170.0
NMB	-0.01%	5.3%	1.7%
MAE	3.2	1.2	33.4
MFB	-1.1%	2.5%	5.3%
R	0.75	0.1	0.2

Table S24. Validation of meteorological conditions using observational data for coastal sites in January 2017.

Parameter	Temp (Kelvins)	Wind speed (m s ⁻¹)	Wind direction (°)
Observed average	279.2	3.6	192.1
Model average	274.4	4.0	155.5
NMB (%)	-2.7	11.4	-19.0
MAE	4.8	1.0	86.4
MFB (%)	-1.7	15.0	6.6
R	0.77	0.59	-0.39

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