

20 **Contents**

21 **Figure S1.** Passenger vehicles ownership information.

22 **Figure S2.** Model domain and some traffic congestion area stations.

23 **Figure S3.** Weekly variation in total pollutant emissions from passenger vehicles.

24 **Figure S4.** Spatial distribution of daily average pollutant equivalent emission on
25 different days.

26 **Figure S5.** The spatial distribution of total pollutant equivalent emission obtained
27 with the traditional algorithm on a 0.05° grid.

28 **Figure S6.** Comparison of temporal variations between simulated results from the
29 traditional algorithm inventory and observed data.

30 **Figure S7.** Comparison of simulated values and observed values of some stations.

31 **Table S1.** Emission factors for each emission standard for 5 pollutants.

32 **Table S2.** Some samples of the original ride-hailing big data.

33 **Table S3.** Detailed information on speed correction curve (SCC).

34 **Table S4.** Deterioration coefficient and sulfur content coefficient of CO, VOC and
35 NO_x of passenger cars.

36 **Table S5.** The main physical and chemical schemes adopted in WRF-Chem in this
37 study.

38 **Table S6.** Passenger vehicle emissions at the province-level in 2019.

39 **Table S7.** Simulation validation results.

40

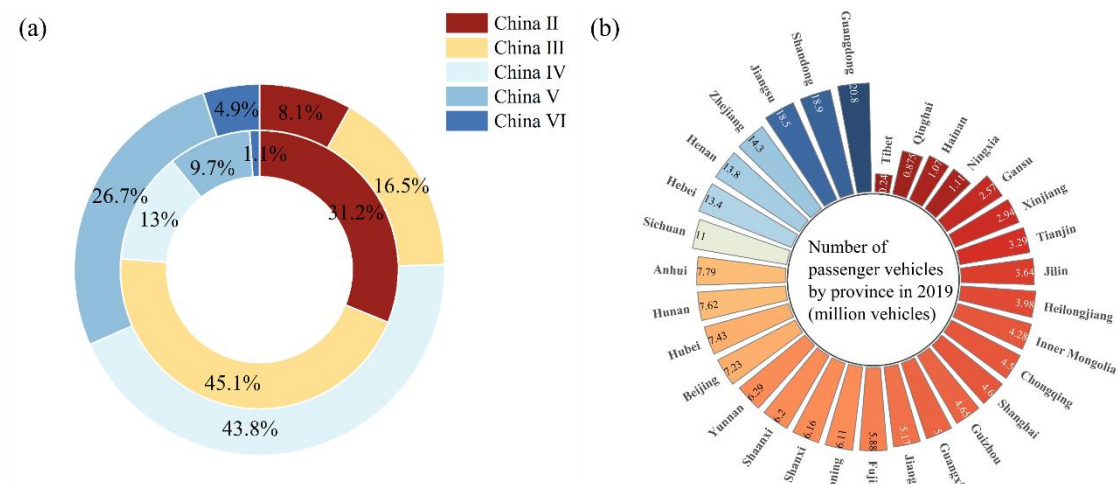


Figure S1. Passenger vehicles ownership information: (a) Percentage of vehicle ownership by emission standard (inner ring is for mini vehicles, outer ring is for small vehicles) and (b) distribution of passenger vehicles ownership by province.

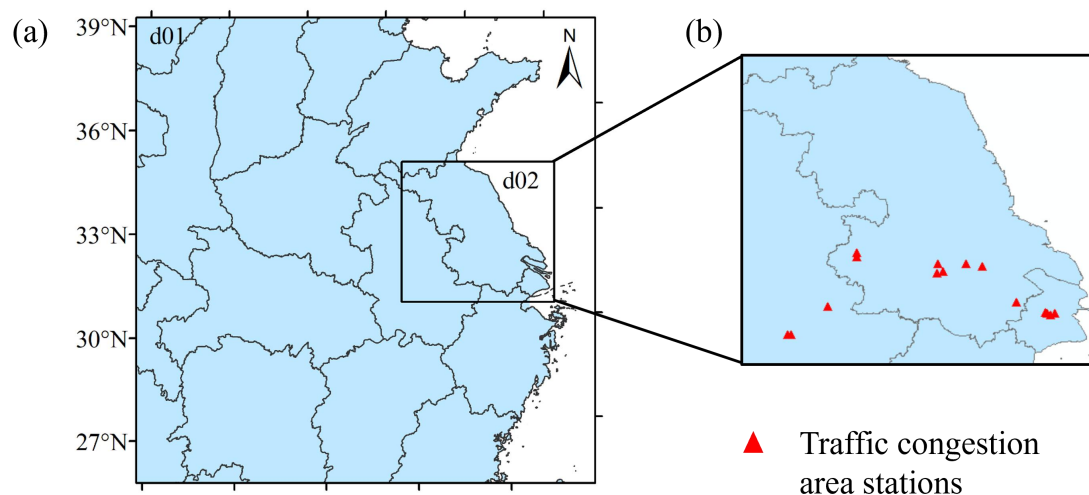


Figure S2. Model domain and some traffic congestion area stations.

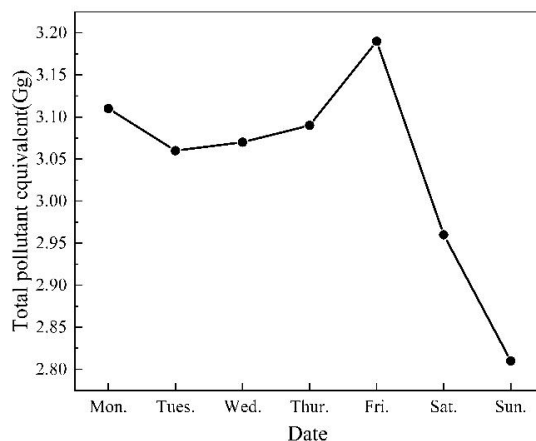


Figure S3. Weekly variation in total pollutant emissions from passenger vehicles.

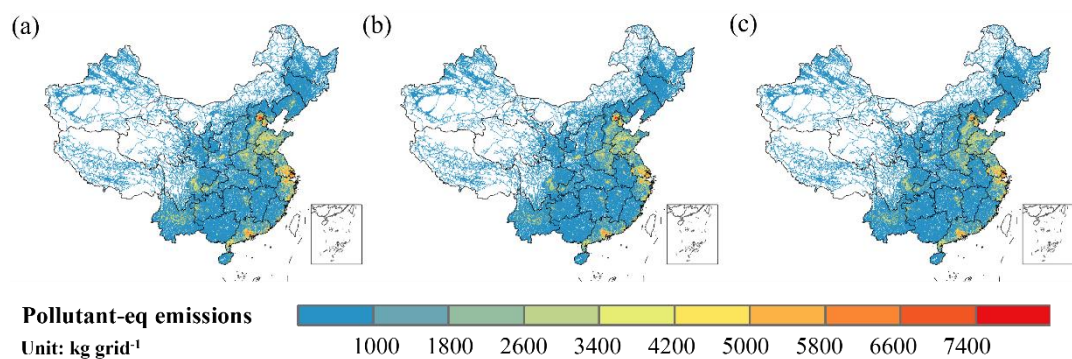


Figure S4. Spatial distribution of daily average pollutant equivalent emissions on different days: (a) Workday; (b) Weekend; (c) Holiday.

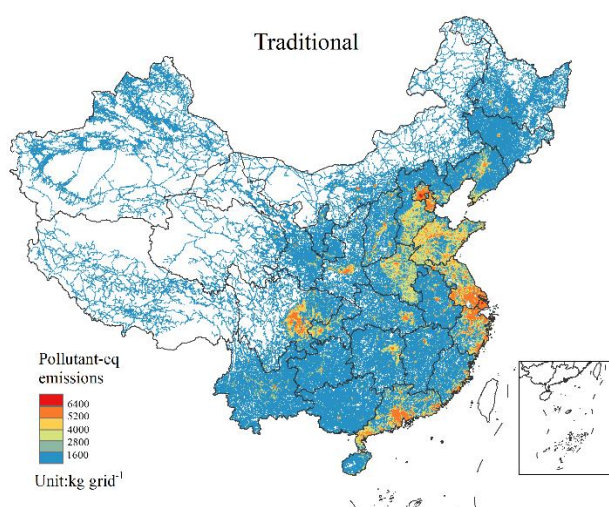


Figure S5. The spatial distribution of total pollutant equivalent emissions obtained with the traditional algorithm on a 0.05° grid.

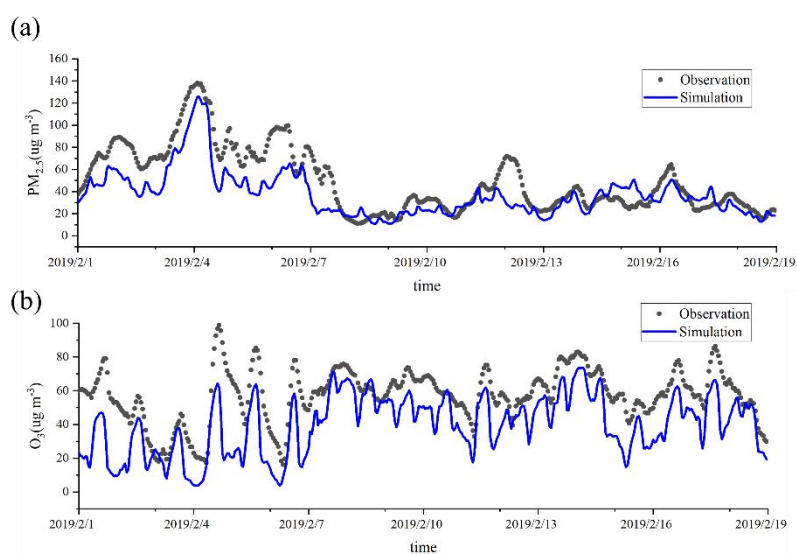


Figure S6. Comparison of temporal variations between simulated results from the traditional algorithm inventory and observed data. (a) PM_{2.5}; (b) O₃.

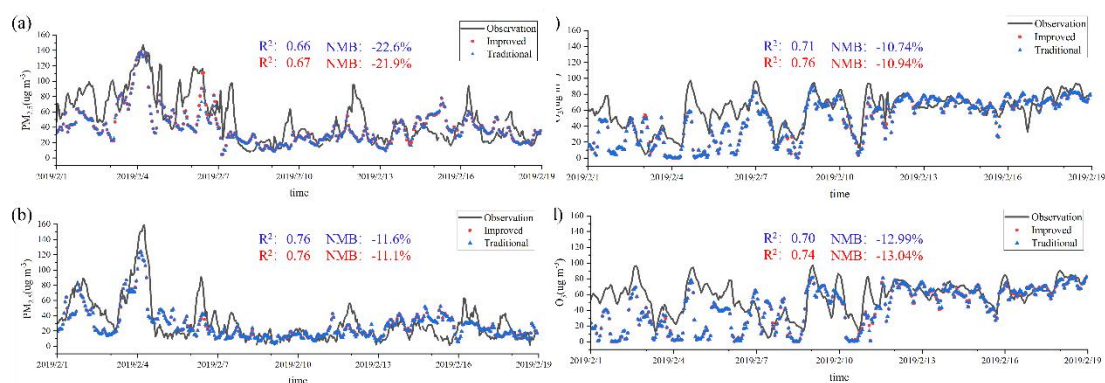


Figure S7. Comparison of simulated values and observed values of some stations: (a) the Administrative Center Monitoring Station, (b) the Putuo Monitoring Station, (c) Pudong Chuansha Monitoring Station, (d) Xinghu Park Monitoring Station.

Table S1. Emission factors for each emission standard for 5 pollutants. (unit: g km⁻¹)

	China II	China III	China IV	ChinaV	ChinaVI	References
CO	6.19672	2.44	1.5645	0.68852	0.4918	Wen et al.(2023)
VOCs	1.4	0.825	0.45	0.25	0.075	Wen et al.(2023)
NO _x	0.32	0.1	0.03	0.02	0.02832	GEI(2014)
PM	0.0022	0.0011	0.0011	0.0014	0.0015	EEA(2019)
NH ₃	0.1043	0.0342	0.0341	0.0123	0.0123	EEA(2019)

*EEA: European Environment Agency

Table S2. Some samples of the original ride-hailing big data.

	Vehicle 1	Vehicle 2	Vehicle 3
Vehicle ID	10533644	12010817	12917912
Longitudes	112.86	110.034153	106.584487
Latitude	22.55783	20.9435499	29.161466
Speed	10.6	57.0	61.0
Direction	184.0	4.0	171.0
Send time	2019-10-01 00:29:32	2019-10-01 00:29:32	2019-10-01 00:29:33
Receive time	2019-10-01 00:29:36	2019-10-01 00:29:36	2019-10-01 00:29:36
Road name	Shenzhou-haiyang Expressway	S113	Lanhai Expressway
Road type	1	4	1

68

Table S3. Detailed information on speed correction curve (SCC).

Pollutant	Speed correction curve (SCC)
CO	$0.00040V^2 - 0.0545V + 2.25$
VOCs	$0.00042V^2 - 0.0565V + 2.27$
NO _x	$0.00020V^2 - 0.0254V + 1.61$
PM	$0.00042V^2 - 0.0565V + 2.27$

*The speed correction curve in this study is referred to Sun et al (Sun et al., 2020).

Table S4. Deterioration coefficient and sulfur content coefficient of CO, VOC and NO_x of passenger cars.

Correction factor	Small			Minicar		
	CO	VOCs	NO _x	CO	VOCs	NO _x
Deterioration coefficient	1.13	1.04	1.21	1.33	1.15	1.60
Coefficient of sulfur content	1.03	1.03	1.02	1.18	1.14	1.09

*The formulae and reference values for the deterioration factor are derived from EEA(2019) and Coefficients of sulfur content are obtained from GEI(MEE, 2014).

* "Small" and "Minicar" are the classifications of passenger cars in China Statistical Yearbook(NBS, 2020).

Table S5 The main physical and chemical schemes adopted in WRF-Chem in this study.

Parameterized options	Parameterization scheme
Cloud microphysics	Morrison 2-moment
Long-wave radiation	RRTMG
Short-wave radiation	RRTMG
Cumulus	Grell-Freitas ensemble
Boundary layer scheme	YSU
Chemistry option	CBMZ
Aerosol option	MOSAIC
Photolysis scheme	2 Fast-J

76

Table S6. Passenger vehicle emissions at the province-level in 2019. (Unit: t)

	CO	VOCs	NO _x	NH ₃	PM
Beijing	229.305	53.175	13.082	3.344	0.075

Tianjin	79.327	18.504	4.698	1.421	0.028
Hebei	220.816	56.646	11.144	4.656	0.113
Shanxi	130.817	34.684	7.611	2.412	0.055
Inner Mongolia	80.231	21.992	4.425	1.504	0.035
Liaoning	111.504	28.648	5.724	2.194	0.050
Jilin	69.545	18.090	3.460	1.329	0.030
Heilongjiang	77.073	20.381	3.485	1.392	0.035
Shanghai	104.048	24.886	5.212	1.786	0.047
Jiangsu	318.876	78.138	16.111	6.628	0.156
Zhejiang	295.723	70.470	14.658	5.293	0.136
Anhui	108.766	27.623	4.954	2.465	0.064
Fujian	100.146	24.155	4.801	2.108	0.052
Jiangxi	71.652	18.374	3.160	1.639	0.042
Shandong	353.804	86.309	18.427	7.066	0.160
Henan	223.515	56.103	10.264	4.563	0.123
Hubei	110.281	29.204	4.655	2.337	0.063
Hunan	105.356	27.600	4.328	2.333	0.063
Guangdong	378.259	86.014	19.357	7.677	0.189
Guangxi	76.229	19.004	3.290	1.591	0.045
Hainan	20.209	4.612	0.956	0.359	0.011
Chongqing	73.161	18.634	3.144	1.466	0.042
Sichuan	207.642	61.195	10.784	3.656	0.102
Guizhou	82.441	25.584	3.968	1.424	0.047
Yunnan	174.648	65.156	13.352	2.202	0.068
Tibet	10.006	4.187	0.894	0.094	0.003
Shaanxi	106.123	28.241	5.163	2.118	0.053
Gansu	62.998	24.705	4.364	0.841	0.023
Qinghai	22.840	10.105	1.613	0.267	0.007
Ningxia	23.528	8.005	1.614	0.387	0.009
Xinjiang	58.930	18.962	3.015	0.927	0.028

Table S7. Simulation validation results of the improved inventory(impr), the traditional algorithm inventory(trad) and meteorological validation.

	R ²	MB	NMB
PM _{2.5} _impr_total	0.850	-14.42	-0.274
PM _{2.5} _impr_holiday	0.839	-21.91	-0.348
PM _{2.5} _impr_normal	0.488	-8.06	-0.205
O ₃ _impr_total	0.771	-18.50	-0.325
O ₃ _impr_holiday	0.764	-17.39	-0.322

O ₃ _impr_normal	0.603	-16.43	-0.281
PM _{2.5} _trad_total	0.850	-14.48	-0.275
PM _{2.5} _trad_holiday	0.839	-22.05	-0.349
PM _{2.5} _trad_normal	0.484	-8.14	-0.207
O ₃ _trad_total	0.68	-18.2	-0.323
O ₃ _trad_holiday	0.76	-17.31	-0.32
O ₃ _trad_normal	0.59	-17.31	-0.28
T	0.95	-0.94	-0.19
Wind speed	0.91	-0.99	-0.29
Wind direction	0.76	-29.03	-0.15

References

- China Statistical Yearbook; NBS (National Bureau of Statistics of China): China Statistics Press, Beijing, 2020.
- EMEP/EEA air pollutant emission inventory guidebook 2019 : technical guidance to prepare national emission inventories.; European Environment Agency: 2019.
- Sun, S., Jin, J., Xia, M., Liu, Y., Gao, M., Zou, C., Wang, T., Lin, Y., Wu, L., Mao, H., and Wang, P.: Vehicle emissions in a middle-sized city of China: Current status and future trends, *Environ. Int.*, 137, 105514, doi:10.1016/j.envint.2020.105514, 2020
- The Announcement about Releasing Five National Technical Guidelines of the Air Pollutant Emissions Inventory., MEE (Ministry of Ecology and Environment), 2014.
- Wen, Y., Liu, M., Zhang, S., Wu, X., Wu, Y., and Hao, J.: Updating On-Road Vehicle Emissions for China: Spatial Patterns, Temporal Trends, and Mitigation Drivers, *Environ. Sci. Technol.*, 57, 14299-14309, doi:10.1021/acs.est.3c04909, 2023