https://doi.org/10.5194/egusphere-2025-5554
Preprint. Discussion started: 28 December 2025

An improved high-resolution passenger vehicle emission inventory for China using ride-hailing big data

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ABSTRACT: As the global automotive industry continues to grow rapidly, the increasing number of passenger vehicles has contributed to worsening air pollution. However, previous studies have insufficiently addressed nationwide hourly vehicle emissions. This study firstly utilized big data of ride-hailing services and traffic flow model to obtain nationwide hourly gridded speed and traffic volume. Then we established a high spatiotemporal resolution (0.01° × 0.01°; 1h) emission inventory by using multiple correction factors. The annual amount of CO, VOCs, NO_x, PM and NH_3 emitted from national passenger vehicles in 2019 were 4087.8, 1069.4, 211.7, 1.9, 77.5 kt, respectively. Despite occupying merely 0.8% of the national territory, urban areas generated 35.3% of the country's total vehicle emissions, due to high local traffic volumes and relatively low vehicle speeds. From a temporal perspective, passenger vehicle emissions exhibit significant holiday effect and weekend effect. In addition, hourly average emissions on workday exceeded those of weekend and holiday by 8 % and 5 % during the morning peak, with these differences increasing to 12% and 18% during the evening peak. Current traditional emission methodology might underestimate emissions by 31.5%. We also used the WRF-Chem model for simulation validation. This hourly-scale inventory provides quantitative support for the precise implementation of pollution control and early warning.

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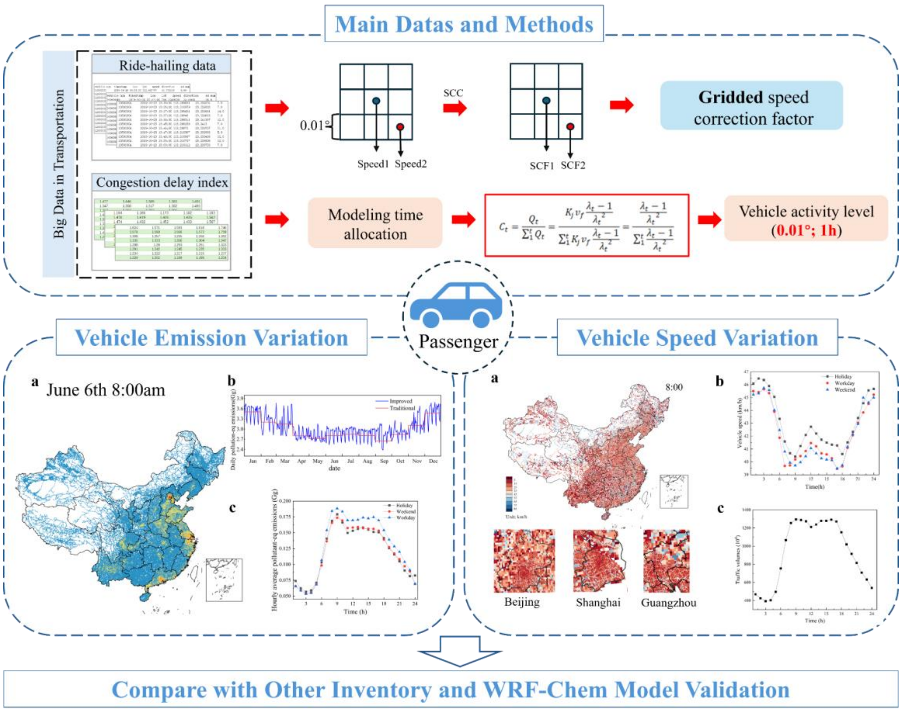

Graphical abstract

1. Introduction

The number of vehicles in China grew from 14.53 million to 260 million over the past two decades, with an average annual growth rate of 16.39%(MEE, 2020a). This growth has driven economic development while adversely impacting air quality and human health(Anenberg et al., 2017). Premature deaths attributable to $PM_{2.5}$ in China amounted to 1.33 million in the year 2020, of which motor vehicle emissions contributed approximately 12.5%(Li et al., 2023b; Luo et al., 2022). In 2019, passenger vehicles accounted for about 80% of the total vehicle population in China (NBS, 2020b) and contributed significantly to vehicular emissions (e.g., VOCs accounted for more than 50% of the total)(Li et al., 2023a). Quantification of passenger vehicle emission characteristics is imperative for the evaluation of relevant emission reduction policies.

With the advancement of regional air quality simulation technology and the increasing demand for atmospheric environmental management, traditional traffic emission statistical methods have become

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inadequate to meet current refined management requirements(Gao et al., 2020). To address this issue, previous studies have developed numerous methods for constructing refined vehicle emission inventories. The first category involves constructing high spatiotemporal resolution traffic emission inventories by using complex emission models, such as COPERT, MOVES, and IVE(Yang et al., 2018; Yu et al., 2021; Wen et al., 2020; Huo et al., 2009). The second category utilizes big data on transportation. For instance, Daniela et al.(Dias et al., 2018) improved the characterization of the spatial variation of vehicle speeds at the city scale through GPS modeling, and Deng et al.(Deng et al., 2020) utilized the BeiDou Navigation Satellite System (BDS) to establish an emission inventory with lower uncertainty for the Beijing-Tianjin-Hebei (BTH) region. However, due to the difficulties in obtaining large-scale and long-term traffic data, most studies are also limited to cities or urban agglomerations, such as Chengdu, Beijing, and the Pearl River Delta (PRD) (Li et al., 2020b; Zheng et al., 2009; Wen et al., 2022), for emission calculations. There is a lack of hourly-resolution emission estimates at the national level.

Emission factors are generally considered to be one of the primary sources of uncertainty in emission inventories(Charis et al., 2010). Many scholars focus merely on the impact of vehicle technology improvements, fuel types, and vehicle aging on emission factors, while often neglecting the influence of speed(Xu et al., 2021; Andrew et al., 2003). Speed has the greater impact on emission factors compared to other correction factors, as it fluctuates dynamically within the same region, while other correction factors remain relatively constant over time. This difference is primarily attributed to variations in engine workload and combustion efficiency at different speeds(Sun et al., 2020; Andrew et al., 2003). The impact of speed on vehicle emissions is both significant and complex. For NO_x, the emission rate of light-duty passenger vehicles at high speeds (>50 km h^{-1}) is 1.6 times that at low speeds (10-20 km h^{-1}), while the emission rates of HC and CO at low speeds are 1.6 times and 2.3 times that of high-speed driving, respectively(Guo et al., 2020). Given this impact, accurate calculation of speed correction factors is important for reducing the uncertainty of emissions factors.

The temporal allocation method can also directly affect the accuracy of high-resolution emission inventories. Previous studies have established emission inventories at monthly scales(Zheng et al., 2014; Jiang et al., 2020; Zhou et al., 2016), or roughly obtained daily-scale data, followed by the construction of a regional-level hourly-scale inventory, such as Biswal et al.(Akash et al., 2022) who systematically analyzed hourly gridded road traffic emissions in Delhi city and Sun et al.(Sun et al., 2021) who considered the influence of the vehicle age-annual average mileage curve and estimated hourly emission

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on a 0.01° × 0.01° grid in Tianjin. However, they have ignored the fluctuations in daily emissions caused by workday, weekend, and holiday, which has significant uncertainty.

To address these gaps, this study aims to improve the accuracy of emission estimations by utilizing big data of ride-hailing services to obtain nationwide speed distribution on a 0.01° grid for the first time and apply it to the speed correction of emission factors. We construct a high spatiotemporal resolution (0.01° × 0.01°; 1h) emission inventory of atmospheric pollutants from passenger vehicles in China in 2019 by further integrating traffic flow models and big data of the congestion delay index. The study also explores the spatiotemporal characteristics of pollutant emissions from passenger vehicles, compares the results with traditional calculation methods, and further evaluates the inventory improvement using WRF-Chem model.

2. Data and methodology

2.1. Estimation of emission inventories

The emission inventory for each pollutant (CO, VOCs, NO_x, PM, NH_3) for passenger cars was estimated with the following equation:

$$E_j = \sum_{i,p,k,t} V_{p,i,k,t} \times BEF_{p,j} \times \varphi_{p,i,j,t} \times \gamma_{p,i,t} \times \lambda_{p,j} \times \theta_{p,j} \times 10^{-9} \quad (1)$$

$$V_{p,i,k,t} = VP_{p,i,k,t} \times VKT_{p,i,t} \quad (2)$$

$$TPE_s = \sum_j \frac{E_j}{PEV_j} \quad (3)$$

In Eq.(1) and Eq.(2), E represents pollutant emissions, t; i represents the grid; j represents the pollutant type, including CO, PM, VOCs, NO_x and NH_3; k represents the vehicle type, including small passenger cars and mini passenger cars; p represents the province; VP, VKT, and BEF represent the vehicle population, annual average vehicle kilometers traveled and baseline emission factors, with units of vehicles, km per year, and g km-1, respectively. φ is the environmental correction factor (including temperature correction factor, humidity correction factor, and altitude correction factor); γ is the speed correction factor; λ is the deterioration correction factor; θ represents other correction factors (including sulfur content correction factor and ethanol blending correction factor). In Eq.(3), TPEs represents the total pollutant equivalents (For assessing the extent of environmental and techno-economic hazards posed by various pollutants), and PEV represents the pollutant equivalent value(MEE, 2018). This study adopted the VKT values for LDPVs in 2019 from the research of Ma et al.(Ma et al., 2022). By utilizing

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data from the China Statistical Yearbook from 2004 to 2019, the lifetime curve of passenger vehicles was obtained, which further yielded the proportion and total amount of passenger vehicles under each emission standard in each province in 2019 (Figure S1). The baseline emission factors were obtained based on other literature (Wen et al., 2023; MEE, 2014; EEA, 2019), with specific details provided in Table.S1.

2.2. Quantification of high-resolution emission factors based on big data of ride-hailing

2.2.1 Gridded speeds and determination of their correction factors

A total of 23.6 billion vehicle trajectory data were collected in this study from Amap Ride-hailing Platform(https://dache.amap.com/amap_mini#/), including workdays (September 24th, October 23rd), weekends (September 28th, October 26th) and holidays (September 13th, October 1st) (Table S2). Based on the vehicle speed data from these days, we assumed that the vehicle speeds on other dates did not vary significantly compared to these representative days. Each vehicle sent data every 3 seconds. Using Python, we processed the data to obtain hourly resolution vehicle speeds on a 0.01° grid. Finally, we obtained gridded hourly vehicle speeds for three representative days: workdays, weekends, and holidays.

Furthermore, we adopted the improved speed correction curve (SCC) method proposed by Sun et al.(Sun et al., 2020) to obtain continuous speed correction factor values for VOC, NO_x, and CO, ultimately resulting in gridded speed correction factors. For specific SCC of various pollutants, please refer to Table.S3.

2.2.2 Corrections for other emission factors

In the equations, φ utilizes daily temperature, humidity, and elevation data, all obtained from ERA5 (https://cds.climate.copernicus.eu/datasets). The deterioration correction factor λ is calculated using relevant equations and coefficients from the EEA.(2019) θ includes the sulfur content correction factor and the ethanol blending correction factor, which are based on the corresponding values from GEI(MEE, 2014). Specific values can be found in Table.S4.

2.3. High-resolution vehicle activity level data combined with traffic flow models

For time allocation for vehicle activity levels, the following formula can be used:

$$V_{p,t,k} = C_{p,t} \times V_{p,k} = C_{p,t} \times VP_{p,k} \times VKT \tag{4}$$

where $V_{p,t,k}$ is the vehicle activity level of model k in province p in time period t; $V_{p,k}$ is the number

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of vehicles of model k in province p.

Cp,t is the time allocation coefficient of province p at time period t. It is obtained by combining the congestion delay index obtained from Baidu Map Traffic and Travel Big Data Platform (https://jiaotong.baidu.com/) with the three-parameter model of traffic flow(Jinping et al., 2024), which is constructed as follows:

The congestion delay index is defined as the ratio of the actual time spent by residents on one trip to the time spent in a smooth state when the travelling distance is the same, and its calculation formula is:

$$\lambda = \frac{T}{T_f} = \frac{\frac{L}{v}}{\frac{L}{v_f}} = \frac{v_f}{v} \tag{5}$$

Where, λ is the congestion delay index; T is the actual time spent travelling; T_f is the time spent travelling at the smooth speed; L is the length of the road section, v is the actual travelling speed, and v_f is the smooth speed of the vehicle, then:

$$v = \frac{v_f}{\lambda} \tag{6}$$

Combined with the basic three-parameter model of traffic flow, the relationship between flow rate and congestion index can be derived:

$$Q = K_j\left(v - \frac{v^2}{v_f}\right) = K_j\left[\frac{v_f}{\lambda} - \frac{\left(\frac{v_f}{\lambda}\right)^2}{v_f}\right] = K_j v_f \frac{\lambda - 1}{\lambda^2} \tag{7}$$

Where Q is the flow rate; λ is the congestion delay index; K_j is the congestion density; v_f is the unimpeded vehicle speed, and K_j and v_f are constants.

In turn, we obtain the formula for calculating the time allocation coefficient of motor vehicle emissions:

$$C_t = \frac{Q_t}{\sum_1^t Q_t} = \frac{K_j v_f \frac{\lambda_t - 1}{{\lambda_t}^2}}{\sum_1^t K_j v_f \frac{\lambda_t - 1}{{\lambda_t}^2}} = \frac{\frac{\lambda_t - 1}{{\lambda_t}^2}}{\sum_1^t \frac{\lambda_t - 1}{{\lambda_t}^2}} \tag{8}$$

Where C_t is the motor vehicle emission time allocation coefficient; t is time; and Q_t denotes the volume of traffic in time period t.

Regarding the spatial allocation of the vehicle activity level, this study was done using the road length data provided by Golder Maps as an allocation index(Gómez et al., 2018), and the gridded vehicle activity level at 0.01° × 0.01° resolution was calculated according to the following formula:

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$$V_{p,i,k,t} = \frac{L_{p,i}}{\sum_i L_{p,i}} \times V_{p,t,k} \tag{9}$$

where $V_{p,i,k,t}$ is the activity level of model k in the i grid of province p in time period t; $V_{p,t,k}$ is the number of vehicles of model k in province p in time period t; and $L_{p,i}$ is the length of the road in the i grid of province p.

2.4 WRF-Chem model setting

To verify the superiority of the improved inventory, this study employed the WRF-Chem model to simulate the atmospheric concentrations of $PM_{2.5}$ and O_3 in the Jiangsu and Shanghai regions (longitude range: 117.5°E ~ 122.0°E; latitude range: 30.0°N ~ 35.10°N) from February 1, 2019 to February 18, 2019 (covering the Spring Festival period and the subsequent week). A two-layer nested model with spatial resolutions of 9×9 km and 3×3 km, respectively, was adopted for the simulation. The specific simulated region is illustrated in Figure S2(a).

The inventory developed in this study was used as the input data for traffic sources, while data from the ABaCAS database was adopted for other emission sources; these two sets of data were jointly utilized to generate the anthropogenic emission files required for the WRF-Chem model(Li et al., 2023a). The 1°×1° Final Operational Global Analysis (FNL) data provided by the National Centers for Environmental Prediction (NCEP, https://rda.ucar.edu/datasets/ds083.2/) was used to obtain the initial meteorological conditions and boundary conditions. Real-time biomass burning emissions were derived from the Fire Inventory from NCAR (FINN, https://www2.acom.ucar.edu/modeling/finn-fire-inventory-ncar). The global simulation results from CAM-Chem (https://www.acom.ucar.edu/cam-chem/cam-chem.shtml) were employed as the initial chemical conditions and boundary conditions. The specific parameterization schemes are presented in Table S5.

This study used observational data from national monitoring stations within the study area to evaluate the simulation results of the emission inventory developed in this study and the traditional inventory, as well as the improvement effects at stations in the top 20% by road density. The simulation results were verified by calculating the normalized mean deviation (NMB) and Correlation Coefficient (R).

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3. Results and discussion

3.1. Spatiotemporal variation of vehicle speed and traffic flow

Vehicle speed and traffic volume are important parameters for describing vehicle driving conditions and traffic flow characteristics. The nationwide average passenger vehicle speed was 42.42 km h^{-1}. The high concentration of work and business activities in the eastern China during the daytime, combined with its large vehicle population, led to generally slower vehicle speeds at 8:00 compared to 22:00. Especially in the key cities such as Beijing, Shanghai, and Guangzhou, city vehicle speeds at 8:00 a.m. typically were 36.4±0.3 km h^{-1} due to significantly increased traffic flow during the morning peak and the circular radial road network which might concentrate traffic flow(Liu et al., 2018). Specific to the road, the average driving speeds were higher on national highways (8:00: 67.12 km h^{-1}; 22:00: 68.59 km h^{-1}), national roads (8:00: 40.05 km h^{-1}; 22:00: 42.92 km h^{-1}), and provincial roads (8:00: 38.18 km h^{-1}; 22:00: 41.46 km h^{-1}) compared to other types of roads (Fig.1a and Fig.1b). During the off-peak period at 22:00, differences in traffic flow speeds across various road types were more apparent. The vehicle speeds on some provincial and county roads had increased significantly. This reflected the non-uniformity of traffic flow distribution(Guan et al., 2024).

There were also differences in average vehicle speeds between provinces, with Inner Mongolia, Jiangxi, and Qinghai having higher speeds (Fig.1c). While Yunnan Province had the lowest average vehicle speed, which might be related to its unique topography. Approximately 94% of Yunnan Province was mountainous, with an average elevation exceeding 2,000 meters(Zhijia et al., 2016). These complex topographical conditions influenced the actual driving speed of vehicles(Hou et al., 2019). In addition, compared to the Northeast China (NE: 8:00: 44.18 km h^{-1}; 22:00: 48.37 km h^{-1}), the average vehicle speeds in the Northwest China (NW: 8:00: 36.89 km h^{-1}; 22:00: 40.41 km h^{-1}), the East China (EC: 8:00:39.89 km h^{-1}; 22:00: 44.56 km h^{-1}), and the South China (SC: 8:00: 40.45 km h^{-1}; 22:00: 44.16 km h^{-1}) regions were lower, due to the NE was predominantly characterized by plains, and its population and transportation network were not as dense as those in the CC and SC (Fig.1c)(Xu et al., 2023).

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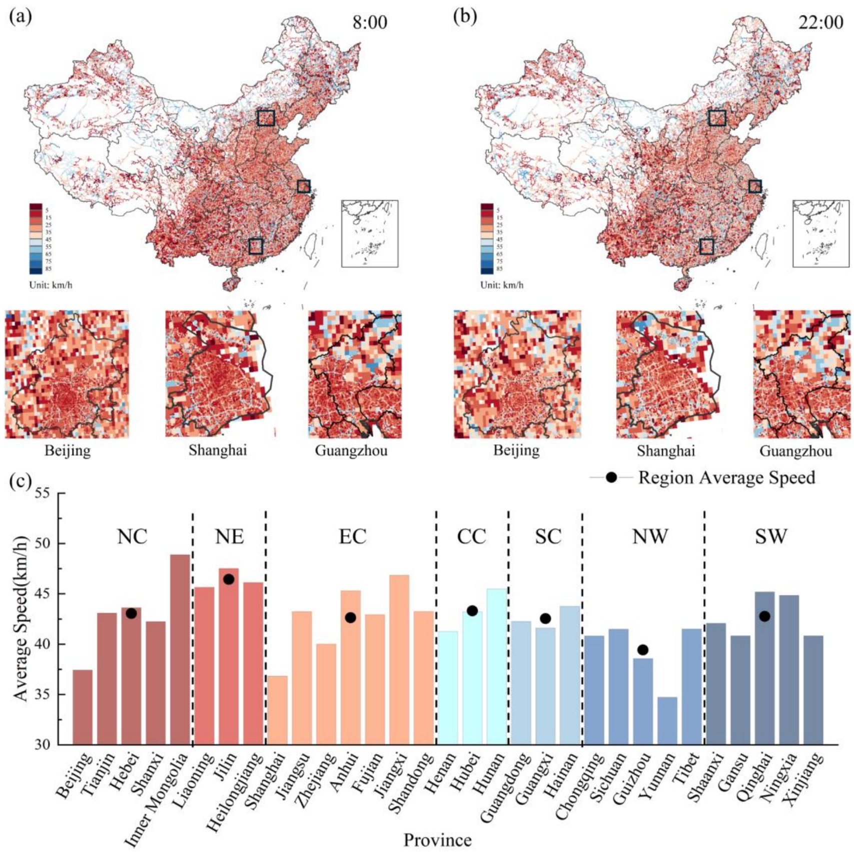

Figure 1. Average speed in China: Spatial distribution of speeds on a 0.01° grid at (a) 8:00 and (b) 22:00 ; (c) Average speeds of provinces and regions, where NC: North China; NE: Northeast China; EC: East China; CC: Central China; SC: South China; NW: Northwest China; SW: Southwest China.

Based on ride-hailing big data, the average speed of passenger vehicles fluctuated across different times. The daily average traffic speeds on workday and weekend were consistent, with both lower than on holiday, at 42.108, 42.111, and 43.032 km h^{-1}, respectively. The higher holiday speed (Fig.2c) can be attributed to reduced urban congestion resulting from increased public transportation use for leisure travel on holidays(Zhang and Gao, 2023b). All three-day types exhibited two low-speed valleys from 7:00-9:00 and 17:00-19:00, with the workday morning valley occurring one hour earlier compared to weekend, consistent with findings by Yang et al.(Yang et al., 2017). The national average speed frequency distribution differed at 8:00 and 22:00 on workday (Fig.2a and Fig.2b), primarily concentrated at 22.07±0.2 km h^{-1} and 44.59±0.3 km h^{-1}, respectively. The large difference in speed between these two

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periods is due to the variation in traffic volumes, as illustrated by the inverse relationship between hourly traffic volume and speed distribution (Fig.2d).

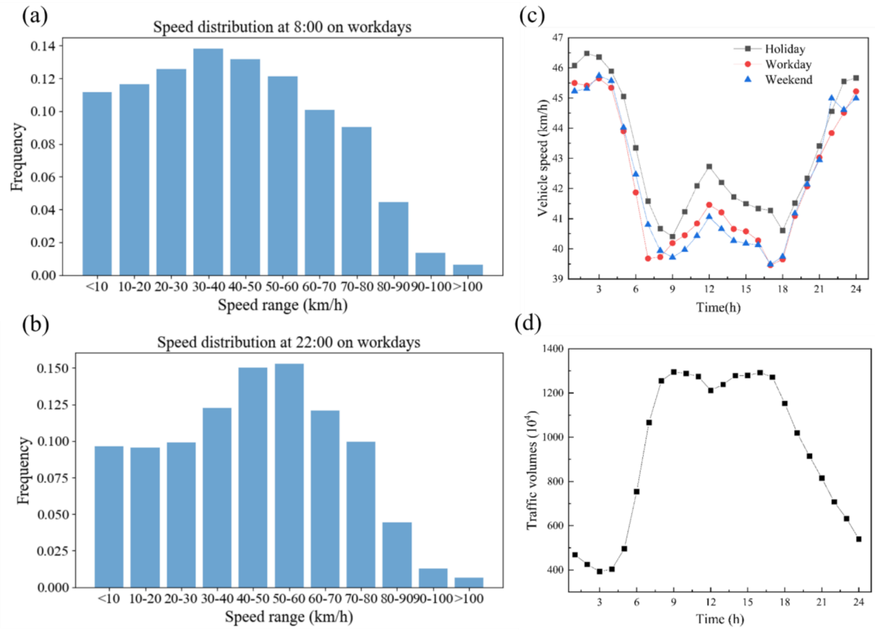

Figure 2. Characteristics of speed and traffic volume changes: speed distribution at (a) 8:00 and (b) 22:00 on workdays; (c) Hourly speed variation on weekend, workday and holiday and (d) hourly traffic volume variation.

3.2. Total passenger vehicle emissions in 2019

The annual amount of CO, VOCs, NO_x, PM and NH_3 emitted from national passenger vehicles in 2019 were 4087.8, 1069.4, 211.7, 1.9, 77.5 kt, respectively and TPEs was 1.6×10^3 kt. Considering these pollutants exhibited similar emission patterns, this study focused on analyzing the total pollutant equivalent emissions. Pollutant emissions from passenger vehicles showed significant spatial heterogeneity. Urban areas, despite occupying only 0.8% of the country's total land area, accounted for a high 35.3% of total vehicle emissions. High-pollution areas mainly concentrated in four urban agglomerations (BTH、YRD、PRD、SCB) (Fig.3a). These areas were densely populated with high vehicle usage frequency, contributing significantly to the total emissions at 48.54%. Specific emissions by province are shown in Table S6. The urban emission density of vehicles within four urban agglomerations was significantly higher compared to rural areas (Fig.3b), as most passenger vehicles primarily operated in urban(Loder et al., 2019).

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This study conducted a comparative analysis of the results from different studies to verify the accuracy of the emission inventory. Compared with previous research results, this research considered the impact of vehicle driving speed on emissions and the differences in emissions between holiday, workday, and weekend, and its estimated emissions in this study fell within the ranges of other estimation results (Table 1).

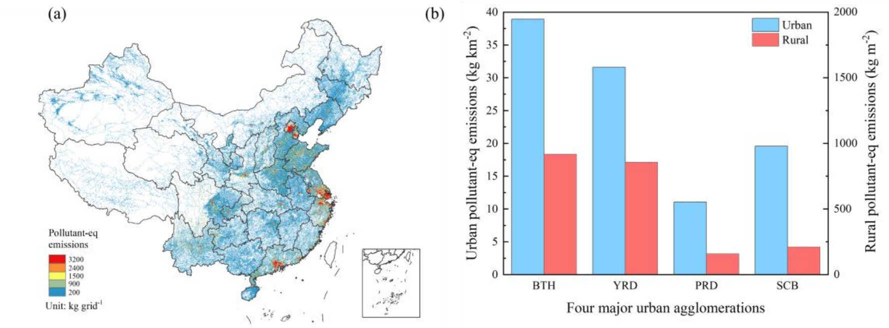

Figure 3. Geospatial distribution of passenger vehicle emissions and the disparities between urban and rural areas: (a) total pollution-eq emissions (TPEs) at 0.01° × 0.01° resolution and (b) urban-rural differences in vehicle emission densities in four major urban agglomerations (BTH: the Beijing-Tianjin-Hebei region; YRD: the Yangtze River Delta region; PRD: the Pearl River Delta region; SCB: the Sichuan Basin) in 2019.

Table 1 Comparison and validation with previous studies. (Unit: ten thousand tons)

References	Year	CO	VOCs	NO_x	NH_3	PM
This study	2019	408.78	106.94	21.17	7.75	0.195
Liu H et al.(2017)	2015	—	67.4	—	—	—
Li S et al.(2020a)	2017	—	—	—	7.5	—
Li S et al.(2023a)	2019	430	95	26.75	8.9	0.17
MEE(2020a)	2019	456.4	121	25	—	0.1
Qi Z et al.(2023)	2019	625	126	27.5	—	0.21

3.3. Temporal variation of passenger vehicle emissions

3.3.1 Seasonal and daily variation

Analysis of passenger vehicle emissions revealed distinct seasonal patterns across different regions (Fig.4c). Specifically, the PRD experienced higher emissions in summer, while the YRD, BTH, and SCB

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regions had higher emissions in winter (Fig. 4c) (Shao et al., 2009; Jiang et al., 2020; Sun et al., 2022). This high winter emission pattern was primarily attributed to adverse weather conditions, which induced prolonged vehicle idling, and reduced driving speeds(Lu et al., 2019). Moreover, vehicles often needed to turn on additional heating equipment, which increased engine load and consequently affected emissions(Abediasl et al., 2023). Notably, Guangdong recorded the highest emissions (Fig.4a), due to its subtropical climate with approximately 80% relative humidity (Liu et al., 2020)and had a high volume of traffic(Yang et al., 2022; Krotkov et al., 2016).

This study considered the impact of workday, weekend, and holiday on daily emissions. During the Spring Festival and National Day, people opted for public transportation for long-distance travel or returning home at the holiday's onset, resulting in the lowest passenger vehicle emissions on the first day, gradually increasing in the following days (Fig.4b)(Zhang and Gao, 2023b). Passenger vehicle emissions normally exhibited a notable weekend effect, with reduced levels on weekend relative to workday (Fig.S3), and daily average pollutant emissions on holiday were 0.92 times those of workday(Wu et al., 2022; Tong et al., 2020). Specifically at daily emissions, for example, from June 17 to June 22, the BTH, YRD, PRD, and SCB regions exhibited notable differences in emission variations. The YRD and PRD regions experienced emission peaks on Friday, while the BTH reached its highest emission level on Monday, corroborating the findings of Wu et al.(Wu et al., 2022)and Zheng et al.(Zheng et al., 2009).

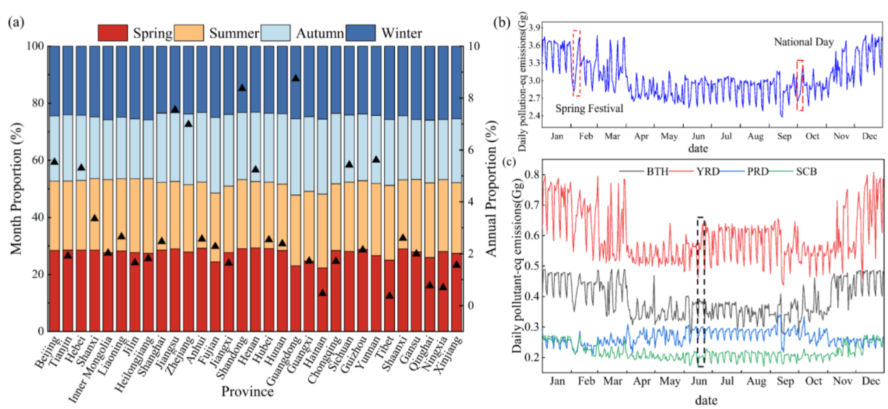

Figure 4. Seasonal and daily scale variations in pollutant emissions: (a) TPEs by province in different months; (b) Daily changes in TPEs across the country and (c) in four major urban agglomerations (BTH, YRD, PRD, SCB).

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3.3.2 Hourly variation

The hourly average TPEs varied among workday, weekend, and holiday (Fig.5a). Peak emission periods were mainly concentrated between 8:00 and 9:00 in the morning and between 16:00 and 17:00 in the afternoon, similar to the daily variation trend of traffic volume(Yang et al., 2019; Shang et al., 2024). During the morning peak, hourly average emissions on workday exceeded those on weekend and holiday by 8% and 5%, respectively, increasing to 12% and 18% during the evening peak. As most private and commercial activities occurred during daylight hours, daytime emissions on workday, weekend, and holiday constituted 85.2%, 84%, and 83.1% of the total daily emissions, respectively.

A distinct variation in the trend of hourly average TPE density is observed across different regions (Fig.5b). The BTH region was highest, followed by the YRD, PRD, and SCB regions. This trend might be related to factors such as traffic conditions, population density, and meteorological conditions in each region(Xie et al., 2019; Yang et al., 2025). The data revealed that the daily average emission densities in the BTH and the YRD were 4.9 times and 4.6 times that of the SCB, respectively. Especially during the peak period at 8:00 in the morning, the hourly average emission densities ratios reached as high as 5.4 times and 5.3 times (Fig.5b). This significant emission difference emphasized the necessity of prioritizing traffic management measures in the BTH region.

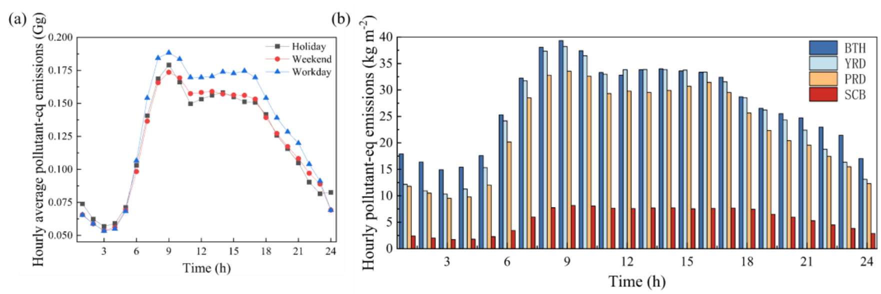

Figure 5. Hourly emission changes for three-day types and regions:(a) hourly total pollutant emission characteristics for weekend, workday and holiday and (b) in four major urban agglomerations (BTH, YRD, PRD, SCB).

3.4. Comparison of passenger vehicle emissions with conventional algorithms

To improve estimation accuracy, this study obtained gridded speed-corrected emission results based on real-time vehicle driving data and compared them with passenger vehicle emission data obtained using traditional methods.

The improved methodology reflected a more accurate and detailed characterization of passenger

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vehicle emissions, which were primarily concentrated in urban centers, with emission intensity gradually decreasing from the city center outwards (Fig.6a) (Jing et al., 2016). Compared to those assumed under steady-state driving conditions in the traditional estimation method, real driving patterns, which might involve more frequent acceleration and deceleration, resulted in higher emissions(Zhang et al., 2023a; Wen et al., 2020). This disparity highlighted the limitations of the traditional algorithm, which underestimated emissions on urban center roads while overestimating emissions on some rural roads outside urban centers (Fig.6a). Overall, the estimation using the traditional method underestimated the total emissions by 31.5%, with Sichuan, Beijing, Shanghai, and Guangdong being underestimated by 43.1%, 38.4%, 29.6%, and 17.4%, respectively. In Tibet, the average vehicle speed stabilized at around 42.5 km h^{-1}, and the SCC analysis revealed a speed correction factor 2.09 times that of the traditional speed correction factor (SCF), leading to the most serious underestimation in this region (Fig.6b)(Sun et al., 2020).

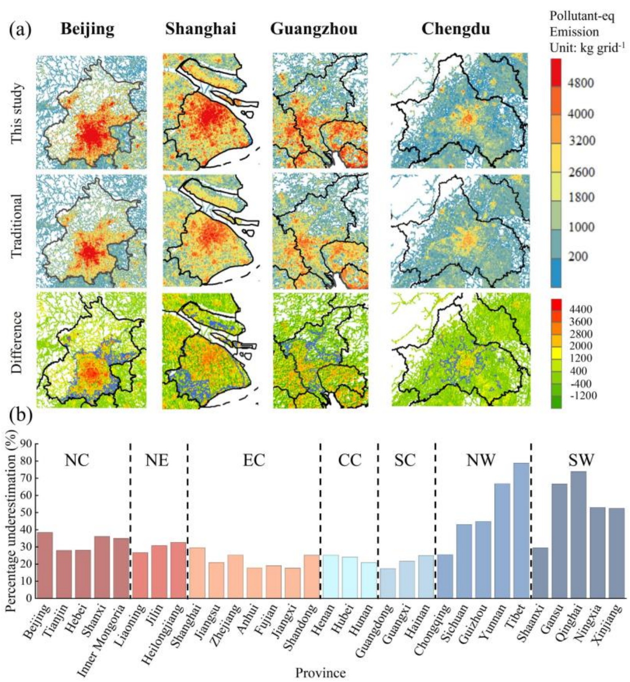

Figure 6. Comparison of this study with traditional algorithms: (a) Beijing, Shanghai, Guangzhou to compare it with the results of the present study (Difference = This Study − Traditional); (b) The percentage of underestimation for each province calculated with the traditional method.

*** The purple boundary is the Urban Growth Boundary (UGB).**

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3.5. Model validation

The simulation results of the inventories reflected the temporal variation of pollutant concentrations well. The improved inventory were more consistent with the observed data from the perspective of hourly change ($PM_{2.5}$: R^2 = 0.850, NMB = -27.4%; O_3: R^2 = 0.771, NMB = -32.5%) (Fig.7 and Fig.S6). The bias might be caused by the underestimation of the input anthropogenic emission inventory, and it fell within an acceptable and reasonable range verified by comparison with other literature (Ma et al., 2018; Wang et al., 2020 and Georgiou et al., 2022). This result indicated that the accuracy of the emission inventory refined through detailed vehicle speed correction was superior to that constructed by traditional algorithms.

The inventory optimization effect was relatively notable in heavily polluted traffic-intensive areas (Fig.S2b), with an overall 0.36% improvement in NMB ($PM_{2.5}$) and 0.02 improvement in R^2 (O_3). This effect is attributable to the complex characteristics of speed fluctuations in these areas. Specifically, the NMB of $PM_{2.5}$ at the Administrative Center Monitoring Station and Putuo Monitoring Station increased by 0.7% and 0.45%, respectively. Meanwhile, the R^2 of O_3 at the Pudong Chuansha Monitoring Station and Xinghu Garden Monitoring Station rose by 0.05 and 0.04, respectively (Fig.S7). However, this study merely achieved a slight improvement, which may be attributed to the small proportion of emissions from passenger vehicles(e.g., approximately 3.2% for CO, 4.7% for VOC, and 1.2% for NO_x)(Li et al., 2023a). The performance of its simulations would be significantly enhanced when the accuracy of vehicle speed correction for the entire traffic source could be further improved.

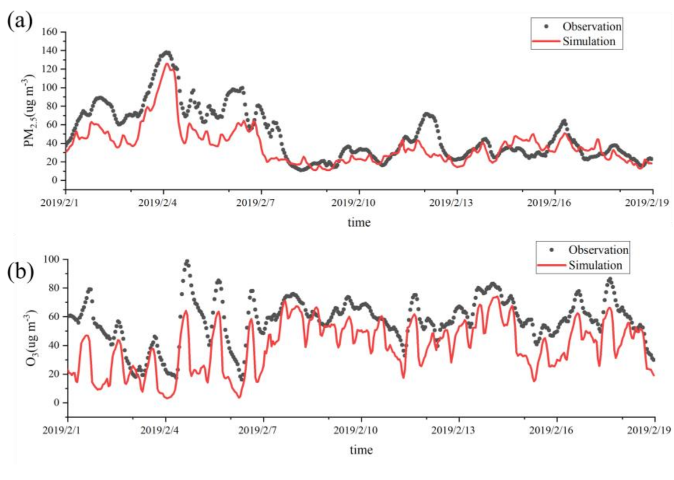

Figure 7. Comparison of temporal variations between simulated results from the improved inventory and

observed data.(a) $PM_{2.5}$; (b) O_3.

4. Conclusions

With the rapid growth of the global automobile industry, the proliferation of passenger vehicles has exacerbated the air pollution problem. Current research lacks a nationwide hourly-scale emissions study for passenger vehicles. Therefore, this study introduces an innovative approach by utilizing big data of ride-hailing services and traffic flow models to obtain nationwide hourly gridded speed and traffic volume, which facilitated the derivation of refined speed correction factors based on actual nationwide driving behavior at both spatial and temporal scales, enabling the construction of a high-resolution (0.01° × 0.01°; 1h) emission inventory for passenger vehicle atmospheric pollutants in China. Our emission inventory revealed that passenger vehicles in China emitted approximately 4087.8, 1069.4, 211.7, 1.9, and 77.5 kt of CO, VOCs, NO_x, PM, and NH_3, respectively, in 2019.

This research showed significant spatial heterogeneity in passenger vehicle emissions in China. Despite occupying merely 0.8% of the national territory, urban areas generated 35.3% of the country's total vehicle emissions. High-pollution areas were predominantly concentrated in four major urban agglomerations (BTH、YRD、PRD、SCB), which contributed significantly to the total emissions at 48.54%，due to high local traffic volumes and relatively low vehicle speeds. Emission density analysis revealed a hierarchical pattern among urban agglomerations, with the BTH region exhibiting the highest density, followed by the YRD, PRD, and SCB regions. And the urban emission density of vehicles within four urban agglomerations was significantly higher compared to rural areas.

Passenger vehicle emissions also exhibit multiscale temporal variations. Higher emissions observed in winter due to weather and driving conditions. In addition, vehicle emissions normally exhibited a notable weekend effect, with reduced levels on weekend relative to workday, and daily average pollutant emissions on holiday were 0.92 times those of workday. There are also differences in the hourly average pollutant emissions across the above three-day types. During the morning peak, hourly average emissions on workday exceeded those on weekend and holiday by 8% and 5%, respectively, increasing to 12% and 18% during the evening peak. Compared with traditional algorithms, this study could more accurately identify the actual emission status of urban roads, reducing the deviation in emission estimation. Current traditional methodology might underestimate by 31.5 %, which is more serious in areas with very little speed variation. The simulated results for $PM_{2.5}$ and O_3 in this study inventory exhibited good

https://doi.org/10.5194/egusphere-2025-5554
Preprint. Discussion started: 28 December 2025

performance.

Our study has limitations in the simulation: the ABaCAS database was adopted herein, as it provides the specific proportion of passenger vehicle emissions. However, compared with the MEIC anthropogenic emission inventory, the NOx and VOCs emissions estimated by this database are underestimated by approximately 20%, which will affect the simulation results to a certain extent. This consequently might results in the underestimation of the simulation results.

Overall, the analytical framework developed in this study accurately quantifies emissions of key atmospheric pollutants from China's passenger vehicle sector. Although the rapid development of vehicle electrification and rail transit is driving a gradual reduction in passenger vehicle emissions, passenger vehicles remain one of the critical sources of pollutants in the transportation sector at the current stage. The “speed-emission” coupling method validated in this study can be extended to transportation sub-sectors such as freight trucks and urban public transport, which effectively improves the accuracy of emission quantification in these fields. To enhance the precision and applicability of our research, more comprehensive big data will be obtained to provide support for the quality of emission inventories. The findings also provide an important scientific basis for intelligent transportation and the formulation of more refined control policies and offer a methodological reference for precise emission management in the transportation sector through its high-resolution data approach.

Associated content

Supporting Information

Figures showing distribution of passenger car ownership; weekly change in emission equivalents; spatial distribution of passenger car emissions for a given three-day period; spatial distribution under conventional algorithms; comparison of simulated values and observed values of some stations and tables showing emission factors for each emission standard; sample data for ride-hailing big data; speed correction curves; deterioration, sulfur correction factors; provincial emissions from passenger cars; parameter settings and verification results of the model simulation.

Acknowledgments

This work was supported by the National Natural Science Foundation of China (42377393), Jiangsu Provincial Young Science and Technology Talents Support Project and Postgraduate Research & Practice Innovation Program of Jiangsu Province(KYCX25_1677).

Author contributions

BL and ZS conceived the study and wrote the paper; BL, ZS, YL, YZ processed the data required for emission estimation and analyzes the processing results; WG, JL, YY, WZ, ZM optimized the research methodology and collected relevant data; HL reviewed the manuscript.

Data availability

For the data used in this work, statements have been included about which data are publically available (accessed through references and links).

Competing interests

The authors declare that they have no conflict of interest.

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