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National-scale emissions, multimedia fate, and future projections of tire-derived 6PPD in China

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Abstract

The tire antioxidant N-(1,3-dimethylbutyl)-N'-phenyl-p-phenylenediamine (6PPD) has emerged as a contaminant of increasing environmental concern because of its widespread use in vehicle tires and the ecological risks associated with its transformation products. However, national-scale assessments linking 6PPD emissions, environmental distribution, and multimedia fate remain largely unavailable for China despite its extensive road network and rapidly growing vehicle fleet. Here, we developed an emission-factor-based framework to quantify 6PPD emissions from vehicle tire wear across 333 prefecture-level cities in China from 2000 to 2020 and coupled these emissions with a multimedia fate model covering 58 secondary river basins. National emissions increased from 0.0064 Mt in 2000 to 0.045 Mt in 2020, with rural roads contributing the largest share of 56.5%. Soil was identified as the dominant receiving compartment, accounting for 57.0% of total environmental loading. Modeled river concentrations agreed well with field observations in major river systems. Multimedia fate analysis revealed that atmospheric degradation and water-air exchange dominated environmental transport, whereas direct atmospheric deposition contributed negligibly. Future projections indicate that annual 6PPD emissions may reach 0.15 Mt by 2060 under the Shared Socioeconomic Pathway 2 scenario. This study provides the first national source-to-receptor assessment of 6PPD in China, offering a quantitative basis for understanding the environmental fate of tire-derived contaminants and supporting future management of 6PPD.

Keywords: 6PPD, Emission, Estimation model, Multimedia fate, Future Projections

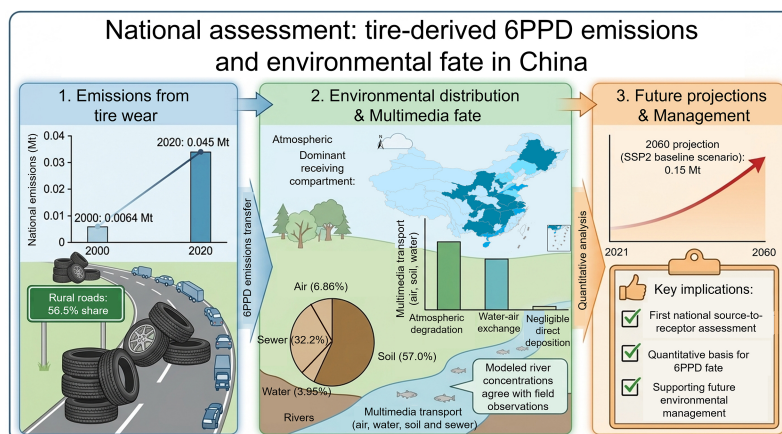
Highlights

- A national source-to-receptor framework was developed for tire-derived 6PPD in China.
- China's tire-derived 6PPD emissions increased seven-fold from 2000 to 2020.
- Soil dominates 6PPD environmental loading and water-air exchange governs transport.
- Rural roads dominated 6PPD emissions, contributing 56.5% of the total.
- Future 6PPD emissions may continue rising through 2060 despite NEV adoption.

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Graphical abstract



Introduction

Non-exhaust traffic emissions have become an increasingly important source of urban environmental pollution. In addition to exhaust gases, road transport continuously generates tire wear particles (TWPs), which contain a complex mixture of functional additives, including antioxidants, vulcanization agents, plasticizers, and their environmental transformation products^[1]. Among these, N-(1,3-dimethylbutyl)-N'-phenyl-p-phenylenediamine (6PPD) has attracted growing attention because it is one of the most widely used tire antioxidants. 6PPD acts as a sacrificial antiozonant by reacting with ambient ozone and other oxidants in the rubber matrix, thereby protecting the tire from oxidative degradation; however, this process can simultaneously generate 6PPD-quinone (6PPD-Q) and other transformation products^[2–4]. During tire abrasion, substantial quantities of 6PPD and its transformation products are released onto road surfaces. These compounds can subsequently be resuspended by wind, retained in roadside soils, transported through stormwater drainage systems, or directly flushed into rivers, resulting in their widespread distribution across air, water, soil, and sediment matrices^[5,6]. Notably, 6PPD-Q and other transformation products have been demonstrated to cause acute mortality in fish and adverse effects on other aquatic organisms^[3,7].

Once released into the environment, 6PPD undergoes complex environmental transport processes. Tire-derived particles deposited on road surfaces can be mobilized through atmospheric dispersion and, more importantly, stormwater runoff, thereby facilitating their transfer from urban environments to riverine and coastal systems^[8]. As a result, river networks function as critical pathways linking terrestrial emissions with downstream aquatic environments, where contaminants may accumulate and persist through continuous inputs from transportation activities^[9–11]. Recent studies have reported the widespread occurrence of 6PPD in road dust, atmospheric particles, surface waters, and sediments, highlighting its ubiquitous distribution in urban environments^[7]. Given its continuous release, extensive environmental occurrence, and strong association with rapidly expanding transportation systems, understanding the sources, environmental distribution, and fate of 6PPD has become an important prerequisite for assessing the impacts of non-exhaust traffic emissions.

China is a valuable and data-rich setting for studying 6PPD emissions and environmental fate at the national scale. Rapid motorization, ongoing road network expansion across diverse terrain, and

marked urban-rural differences in infrastructure, hydrology, and economic development have created strongly heterogeneous spatial patterns of tire-derived chemical inputs^[12,13]. However, existing assessments remain spatially fragmented: published studies have reported local concentration profiles and some provincial emission totals, but a nationally consistent, city-level inventory that is explicitly linked to basin-scale receiving environments is still lacking. This gap constrains reliable risk assessment, because key determinants of 6PPD environmental behavior, such as traffic intensity, impervious surface cover, sewer access, precipitation patterns, and river network density, vary greatly across Chinese regions^[14]. Furthermore, although emission-factor-based and activity-based approaches have been successfully applied in Europe and North America^[1,15,16], these studies generally focus on emission inventories and do not explicitly connect emission sources with basin-scale environmental exposure or multimedia transport processes. Likewise, existing multimedia fate studies often rely on simplified spatial assumptions and therefore cannot adequately capture the strong regional heterogeneity that characterizes China's hydrogeological and climatic conditions^[17]. To date, no study has integrated city-level 6PPD emissions, secondary river-basin boundaries, multimedia fate modelling, and future emission projections within a unified national-scale framework. Consequently, the source-to-receptor relationships governing the environmental distribution of 6PPD remain poorly understood.

To address these knowledge gaps, this study presents a spatially explicit, temporally resolved, and future-oriented source-to-receptor assessment framework for tire-derived 6PPD in China. Specifically, we aimed to: (1) quantify 6PPD emissions across 333 prefecture-level cities from 2000 to 2020 and identify dominant source categories and receiving environmental compartments; (2) link city-scale emissions to 58 secondary river basins and estimate basin-level pollutant inputs and multimedia concentrations; (3) characterize inter-compartment transport fluxes and dominant migration pathways using a multimedia fate model; and (4) project future 6PPD emissions to 2060 under plausible socioeconomic and transportation-transition scenarios. By integrating emission estimation, spatial allocation, multimedia fate modelling, and future scenario analysis, this study establishes the first national-scale source-to-receptor framework for 6PPD in China and provides a scientific basis for understanding and managing tire-derived contaminants in rapidly urbanizing regions.

Materials and methods

Study area and parameter description

The study covered mainland China, encompassing 333 prefecture-level administrative regions in 31 provinces, autonomous regions, and municipalities (excluding Hong Kong, Macao, and Taiwan). Historical emissions were estimated for 2000–2020; projections were extended to 2060. Two complementary spatial units were employed: prefecture-level regions for emission estimation and China's secondary river basins for basin-input and multimedia-fate analysis. The secondary-basin boundaries followed the national industry standard^[18], encompassing 58 secondary basins that span the major hydrological systems of the country. This is specific to the 58 secondary basins corresponding to the first-level basins as defined by China's state departments. Each basin is assigned a serial number to facilitate future research descriptions (Supplementary Figs S1 and S2).

Vehicle ownership and road mileage data by vehicle type and road class were obtained from the National Bureau of Statistics Yearbook (NBSC) (2001–2021) and Provincial Bureau of Statistics Yearbooks (BSC) (2001–2021)^[19]. Unpublished city-level vehicle registration data were obtained from vehicle-management offices through official information-disclosure requests. Annual average vehicle kilometers travelled (VKT) were derived from the 2015 Ministry of Environmental Protection Technical Guidelines for Road Motor Vehicle Emission Inventory of Air Pollutants (Trial) and supplementary literature^[20–22]. The relevant socio-economic indicators used to predict car ownership during 2021–2060 mainly include population, gross domestic product (GDP), per capita GDP, urbanization rate, total retail sales of consumer goods, per capita disposable income of rural households, per capita disposable income of urban residents, highway passenger volume, highway freight volume, highway mileage, total export-import volume, total export volume, and total import volume index data, which are also from NBSC and BSC, and future values of these indicators were taken from the Shared Socioeconomic Pathway 2 (SSP2) dataset^[23,24].

Tire wear emission factors (EFs) and environmental allocation fractions were taken from the International Union for Conservation of Nature (IUCN) framework^[12], which provides road-type- and vehicle-type-specific values widely used for cross-national comparison. The mass fraction of 6PPD in tire rubber (0.4–2%) followed Tian et al.^[7] and provided the minimum and maximum bounds for emission estimates. Physicochemical properties of 6PPD were retrieved from EPIWEB 4.1. Spatial overlay between administrative boundaries and basin boundaries was performed in ArcGIS 10.8.

Emission estimation method

6PPD emissions were estimated as the product of TWP generation and the 6PPD mass fraction in tire rubber, which is the recommended method from the International Union for Conservation of Nature (IUCN)^[25,26]. The IUCN allocation factors describe the mass partitioning of TWPs among environmental compartments (air, soil, sewer, surface water). Their application to 6PPD rests on the assumption that the majority of 6PPD remains embedded within the TWP matrix during abrasion, so that the environmental release pathways of TWP-bound 6PPD follow the same physical mass distribution as TWPs themselves. This assumption is supported by Baensch-Baltruschat et al.^[27] and Wagner et al.^[28], who demonstrated that tire additives are predominantly transported in association with the particle phase. The leached fraction of 6PPD from TWPs into water is estimated to be less than 5% of the total mass under typical environmental conditions^[29,30], confirming that TWP-bound transport is the dominant pathway. For

each prefecture-level region, vehicle type, and road type, TWP generation was calculated using Eqs. (1) and (2):

$$E_{total} = \sum_{road\ type} f_{i/j/k} \times f_{pav} \times \sum_{vehicle\ type} VKT \times EF_{wear} \quad (1)$$

$$E_{i/j/k} = (1 - f_{air}) \times \sum_{road\ type} f_{i/j/k} \times f_{pav} \times \sum_{vehicle\ type} VKT \times EF_{wear} \quad (2)$$

where index i , j , and k represent surface water, soil, and sewer; E_{total} represents the total mass of TWPs; $E_{i/j/k}$ represents the total amount of TWPs discharged into the environment of i , j , and k (unit: 10^{-2} Mt); f_{air} represents the fraction of TWPs in the air; f_{pav} represents the fraction of TWPs available for runoff to adjacent surface water, soil, and sewer, and it is a correction for entrapment in the road. $f_{i/j/k}$ is the compartment-specific allocation factor, which varies by road types. EF_{wear} is the vehicle- and road-specific tire wear emission factor (unit: mg/km). Vehicle types included large, medium, small, and mini passenger cars; heavy, medium, light, and midget trucks; and miscellaneous vehicles. Road types included rural roads, urban roads, and expressways. The model was implemented in Python using the PyTorch framework, enabling sub-second calculation for all 333 prefecture-level regions. Spatial assignment to secondary basins was performed via ArcGIS overlay, and the 6PPD mass within TWPs was determined by calculating the product of the mass fraction of 6PPD and the emissions of TWPs. Detailed estimation models and related parameters are shown in Supplementary Tables S1 and S2 (Supplementary material A) and the Emissions and fate of 6PPD Data Sheet (Supplementary material B).

Multimedia fate modelling

Basin-level 6PPD fate was simulated using a level III multimedia environmental fate model that considers air, water, soil, and sediment compartments, which is based on our previous study^[31]. Generally, prefecture-level 6PPD inputs were aggregated to secondary basins by spatial overlay (Supplementary Tables S3 and S4) and used as model inputs. The model computed steady-state concentrations in each compartment and inter-compartment transport fluxes, including atmospheric deposition (dry and wet), surface runoff, sewer-mediated transfer, sediment-water exchange, and degradation. Compartment volumes, hydrological parameters, and degradation half-lives were obtained from published databases and regional statistics. Physicochemical partitioning was governed by Henry's Law, octanol-water and octanol-air partition coefficients, and organic-carbon-normalized sorption coefficients derived from EPIWEB 4.1. Detailed model descriptions and parameter values are provided in Text S1 and Supplementary Tables S5 and S6 of the Supplementary material A.

Future emission projection

Future 6PPD emissions were driven by projected vehicle ownership. A principal component analysis-back propagation neural network (PCA-BP) model was trained on historical socioeconomic indicators (2000–2015), validated on 2016–2020 data, and applied for projections through 2060 (Supplementary Fig. S3). The aforesaid factors were first analyzed using PCA and the results are summarized in Supplementary Tables S7–S9. PCA identified total national population (X_1), GDP (X_2), per capita GDP (X_3), and urbanization rate (X_4) as the dominant predictors of national vehicle ownership (Supplementary Tables S7–S9).

Fleet composition was adjusted to reflect the anticipated transition toward new energy vehicles (NEVs). Consistent with China's new energy vehicle industry development plan (2021–2035)^[32], NEV sales were assumed to reach 20.0% of all new vehicle sales by 2025 (average annual growth rate 24.1% from 2021 to 2025). Beyond 2025, the adoption trajectory was aligned with the carbon-neutral

energy scenario in Shell's 2060 outlook, under which NEVs account for 80.0% of new sales^[33]. The remaining 20% conventional vehicles were assumed to follow an average annual growth rate of 2.23% from 2026 to 2060. Because tire wear emission factors depend primarily on vehicle-road interaction rather than powertrain type, the same EFs and VKTs were applied to both conventional and new energy vehicles^[34]. The projected deceleration in emission growth after 2050 therefore reflects the anticipated plateau in per-capita vehicle ownership under the carbon-neutral scenario. The predicted future values of EFs and VKT, as well as the estimation model, were the same as the historical values and methods. Detailed future prediction methods are also summarized in [Text S2](#) of the [Supplementary material A](#).

Results and discussion

National emission trends and source contributions of 6PPD

National 6PPD emissions grew continuously from 0.0064 Mt in 2000 to 0.045 Mt in 2020, representing a seven-fold increase at an average annual growth rate of 10.2% ([Fig. 1](#)). The temporal trajectory was not uniform. Emissions accelerated markedly after 2008 in response to macroeconomic policies and rising household income that together propelled rapid vehicle-ownership growth^[34]. From 2009 to 2011, the annual growth rate exceeded 15.0%, pushing total emissions above 0.02 Mt by 2011. After 2012, the pace slowed considerably to 3.76% per year through 2020, consistent with a more mature motorization stage in which market saturation and tightening fuel-efficiency standards dampened marginal additions to the vehicle fleet.

[Figure 1a](#) disaggregates 2020 emissions by road type and vehicle category. Rural roads contributed the largest share, followed by urban roads and expressways, because road mileage and cumulative vehicle-distance are far greater on the lower-grade network than on high-capacity corridors. Within vehicle categories, small passenger cars and heavy trucks were the dominant contributors among passenger and freight vehicles, respectively, reflecting their large fleet size and relatively high per-kilometer tire wear rates. This distribution is important for policy because it implies that emission reduction strategies focused exclusively on highways would miss a substantial portion of diffuse tire-derived inputs from the rural and urban road network.

Environmental partitioning further showed that most 6PPD was released to soil, followed by sewer systems, air, and surface water ([Fig. 1b](#)). In 2020, approximately 57.0% of 6PPD was deposited into soil, 32.2% entered sewer systems, 6.86% was released into air, and only 3.95% directly entered surface water. This hierarchy reflects the physical mechanisms of TWP dispersal: large particles tend to be retained near the road surface or trapped in drainage inlets and accumulate in roadside soils, while fine particles are entrained into stormwater or resuspended in air^[27,35]. The small direct surface-water fraction should not be interpreted as low aquatic relevance, however, because sewer discharge during storms and runoff remobilization from soil can transfer sewer-bound and soil-bound 6PPD to rivers over time. The large sewer fraction specifically indicates that urban drainage infrastructure acts as both a reservoir and a transport conduit, creating episodic aquatic pulses during precipitation events^[36,37].

Spatial distribution of 6PPD emissions across China

The spatial distribution of 6PPD emissions in 2020 showed strong regional heterogeneity ([Fig. 2a](#); [Supplementary Figs S4](#) and [S5](#)). Emissions were highly concentrated in economically developed coastal corridors. The three largest hotspot clusters were: (i) the Beijing-Tianjin-Hebei agglomeration, encompassing China's capital economic circle and 13 major cities; (ii) the Yangtze River Delta agglomeration, covering 41 cities across Shanghai, Jiangsu, Zhejiang, and Anhui; and (iii) the Shandong Peninsula, including eight cities in the lower Yellow River reaches. Collectively, these regions contributed 0.0027–0.014 Mt of emissions, accounting for more than 30.4% of the national total. This spatial pattern is consistent with land urbanization maps^[38]. In addition, inland high-emission centers were limited to major provincial capitals and key transport hubs, such as Xi'an, Chengdu, Wuhan, Zhengzhou, Hefei, and Chongqing. Together with coastal areas, these cities comprised approximately 70.0% of the top-20 emission cities in 2020 ([Supplementary Material B](#)). Overall, the 88 cities in the eastern region (representing 26% of the 333 cities) contributed about 80% of national emissions, highlighting a strong spatial clustering of emission burdens in eastern China. A comparable spatial pattern of TWP emissions has also been observed in China's coastal regions using the empirical formula approach^[13], suggesting that 6PPD deposition associated with TWPs along coastal areas is an emerging environmental concern.

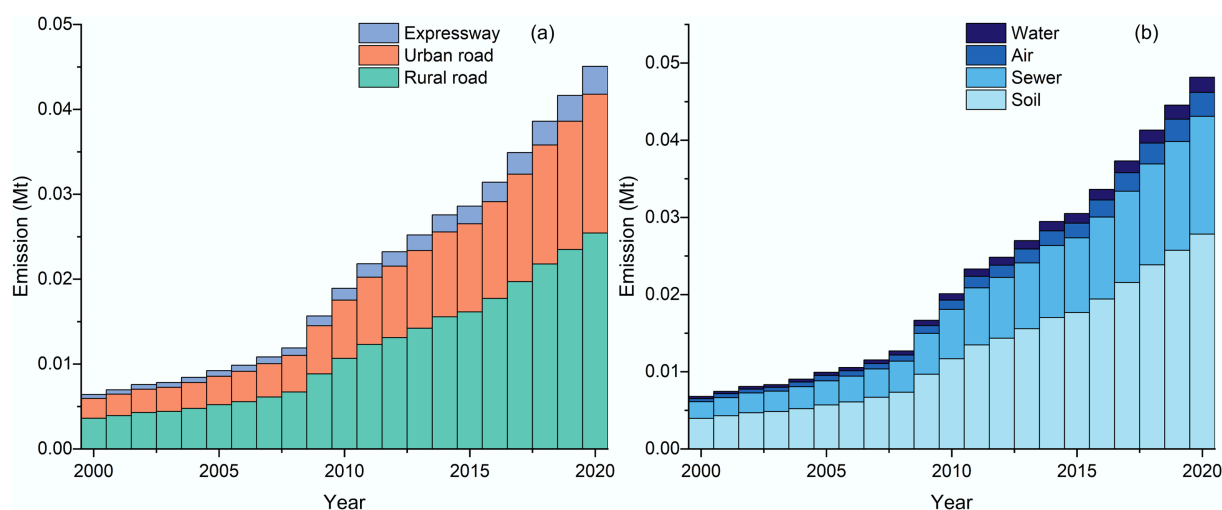


Fig. 1 National 6PPD emissions and environmental partitioning in China. (a) Contribution of road types and vehicle categories to 6PPD emissions in 2020. (b) Environmental compartmental distribution of 6PPD among soil, sewer, air, and surface water in 2020.

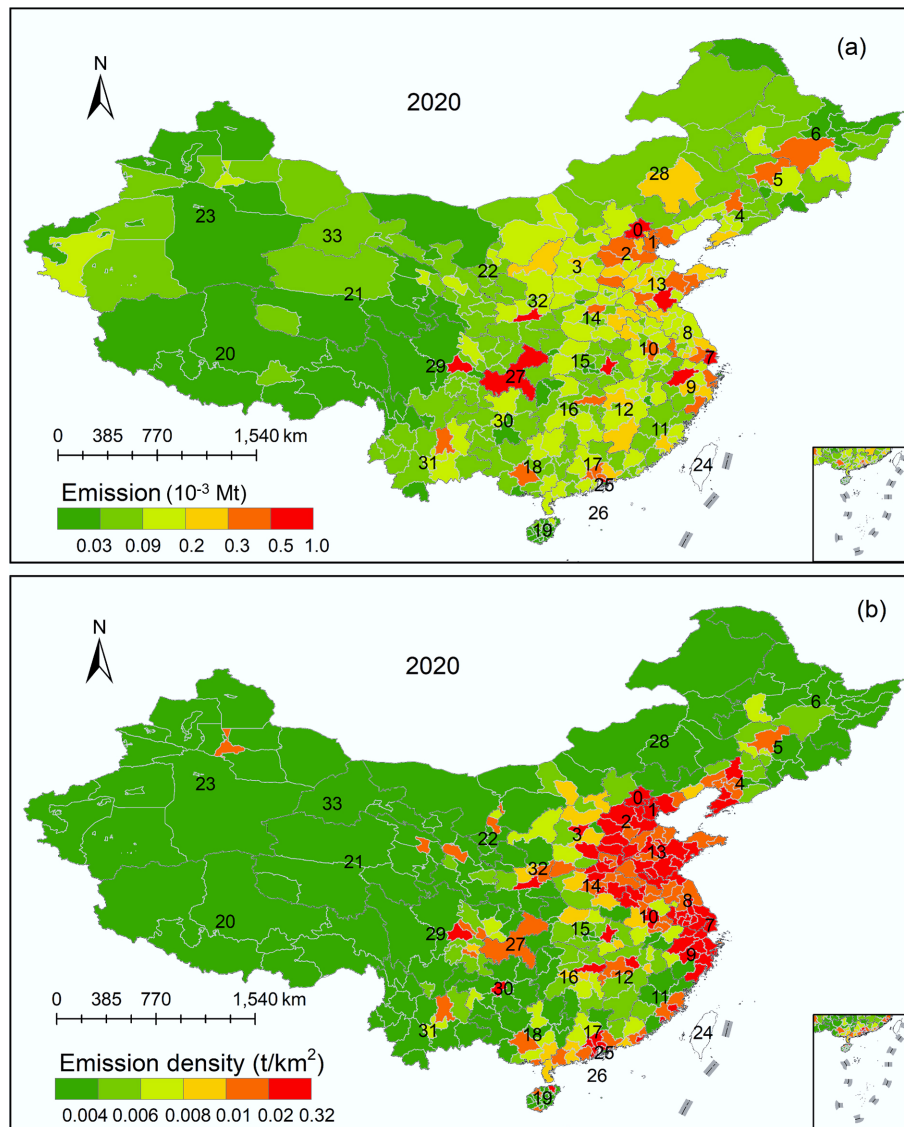


Fig. 2 6PPD emissions distribution in China in 2020. (a) The total emission. (b) The emission density for each region. IDs: 0-Beijing; 1-Tianjin; 2-Hebei; 3-Shanxi; 4-Liaoning; 5-Jilin; 6-Heilongjiang; 7-Shanghai; 8-Jiangsu; 9-Zhejiang; 10-Anhui; 11-Fujian; 12-Jiangxi; 13-Shandong; 14-Henan; 15-Hubei; 16-Hunan; 17-Guangdong; 18-Guangxi; 19-Hainan; 20-Xizang; 21-Qinghai; 22-Ningxia; 23-Xinjiang; 24-Taiwan*; 25-Hong Kong*; 26-Macao*; 27-Chongqing; 28-Inner Mongolia; 29-Sichuan; 30-Guizhou; 31-Yunnan; 32-Shanxi; 33-Gansu. Note: *Geographic reference only, not included in the analysis. This figure is based on the standard map service of the National Platform for Common GeoSpatial Information Services (<http://www.tianditu.gov.cn>), with the map approval number GS(2024)0650. The administrative boundaries remain unmodified.

When normalized by regional area, the spatial pattern of 6PPD emission density (Fig. 2b) revealed even more pronounced regional disparities and concentration. The emission density ranged from 0.004 to 0.32 t/km^2 , spanning nearly two orders of magnitude. The highest emission densities ($>0.02 t/km^2$) were concentrated in the Yangtze River Delta region (Shanghai, Jiangsu, Zhejiang), the Pearl River Delta agglomeration (Guangdong), and parts of the Beijing-Tianjin-Hebei region, corresponding to China's most economically developed and urbanized areas. These regions exhibited emission density values 50–80 times higher than western provinces (Xizang, Qinghai, Xinjiang, Ningxia), which typically showed densities below 0.006 t/km^2 . The emission density pattern directly reflects the underlying relationship between vehicular activity and urbanization levels^[39]. Coastal metropolitan areas with dense road networks, high vehicle ownership rates, and concentrated tire-wear emissions demonstrated the highest densities. Notably, even within high-emission

provinces identified in Fig. 2a, emission density showed substantial spatial heterogeneity—with urban cores significantly exceeding regional averages. This indicates that 6PPD emissions are not uniformly distributed across provinces but rather heavily concentrated in metropolitan regions and transportation corridors.

The spatial pattern confirms that 6PPD behaves as an urbanization-dependent contaminant driven by the co-occurrence of dense road networks, high vehicle ownership, and extensive impervious surfaces^[26,28,40]. This coupling is mechanistically consistent: rapid motorization increases tire abrasion rates; impervious surfaces reduce infiltration and enhance pollutant mobilization; and urban drainage networks accelerate environmental transfer to receiving waters. Principal component analysis of 6PPD emissions against socioeconomic indicators (Supplementary Tables S7–S9) confirmed that urbanization rate, per capita GDP, and total vehicle ownership are the strongest predictors, a finding that aligns with cross-city

observations of 6PPD in PM_{2.5} from five major Chinese megacities^[41]. The implication is that any future scenario projecting further urbanization in currently low-density western cities will tend to create new emission hotspots in regions where stormwater infrastructure and monitoring programs are currently less developed.

Multimedia environmental concentrations of 6PPD in river basins of China

The multimedia fate model produced 2020 steady-state 6PPD concentrations across China's secondary river basins in four environmental compartments (Fig. 3). Simulated concentrations ranged from 8.93×10^{-7} to 1.66×10^{-6} ng/m³ in air, from 0.74 to 1.25 ng/L in rivers, from 60.1 to 66 ng/g in soil, and from 1.24×10^{-9} to 2.33×10^{-9} ng/g in sediments. This distribution pattern is consistent with preferential retention of tire-derived particles in terrestrial compartments adjacent to emission sources, as expected from rapid settling of coarse TWP fractions and strong sorption affinity of 6PPD to organic matter in roadside soils. Spatially, basins with the highest 6PPD concentrations corresponded to those receiving inputs from the most densely populated and heavily trafficked regions (Fig. 3). The Yangtze River system, Yellow River lower reaches, Pearl River system, and coastal basins of eastern China consistently showed elevated concentrations across compartments. In contrast, northwestern and southwestern basins such as the Erqis River, Junggar Inflow Zone, and Qiangtang Plateau basins exhibited lower concentrations, consistent with their sparse road networks and lower vehicle activity.

Model-data comparison provides important validation. Simulated river concentrations for the Pearl River and Dongjiang River (0.989 and 1.02 ng/L, respectively) agree well with field observations of 0.31–1.29 ng/L reported for these systems^[3,42] (Supplementary Table S10). This agreement supports the practical validity of the emission-to-fate linkage for regional exposure characterization. By contrast, concentrations reported in Canada's Don River (300–2,300 ng/L) were 294–2,326 times higher than our simulated Chinese values^[43],

reflecting the more severe impact of tire-derived pollution documented in North American urban watersheds.

Although all simulated concentrations remained below the sublethal threshold of 95 ng/L for silver salmon^[44], potential ecological risks remain. First, basin-averaged steady-state concentrations underestimate peak stormwater-event concentrations, which can exceed annual means by one to two orders of magnitude^[45]. Second, other sources of 6PPD besides tire wear particles, such as various rubber products, can release target substances, increasing the total environmental intake and leading to higher exposure concentrations. Third, since a fraction of emitted 6PPD may undergo transformation to its transformation products, the modeled parent 6PPD concentrations may overestimate actual levels due to the unaccounted reaction loss^[46]. Therefore, the current results should be interpreted as a lower bound on aquatic exposure, and targeted monitoring in urbanized basins during and after storm events remains necessary.

Environmental transport fluxes and dominant migration pathways of 6PPD in basins of China

The multimedia fate model (Fig. 4) reveals that 6PPD undergoes extensive redistribution among air, soil, water, and sediment compartments in Chinese river basins. The overall transport network is dominated by exchanges involving the atmospheric compartment, highlighting the important role of air-mediated transformation and intermedia transfer in regulating the environmental fate of 6PPD. Air degradation (T_{10m}) represents the dominant removal pathway, whereas diffusion from air to water (T_{12d} , T_{12p} , and T_{12w}) and from air to soil (T_{13d} , T_{13p} , and T_{13w}) is comparatively negligible, reflecting limited direct atmospheric deposition and exchange. This pattern suggests that once released from tire wear particles, 6PPD is more likely to undergo local transformation and compartmental cycling than long-range redistribution through atmospheric deposition pathways. Similar multimedia transport behavior has been reported for tire-derived contaminants and tire wear particles in both urban and

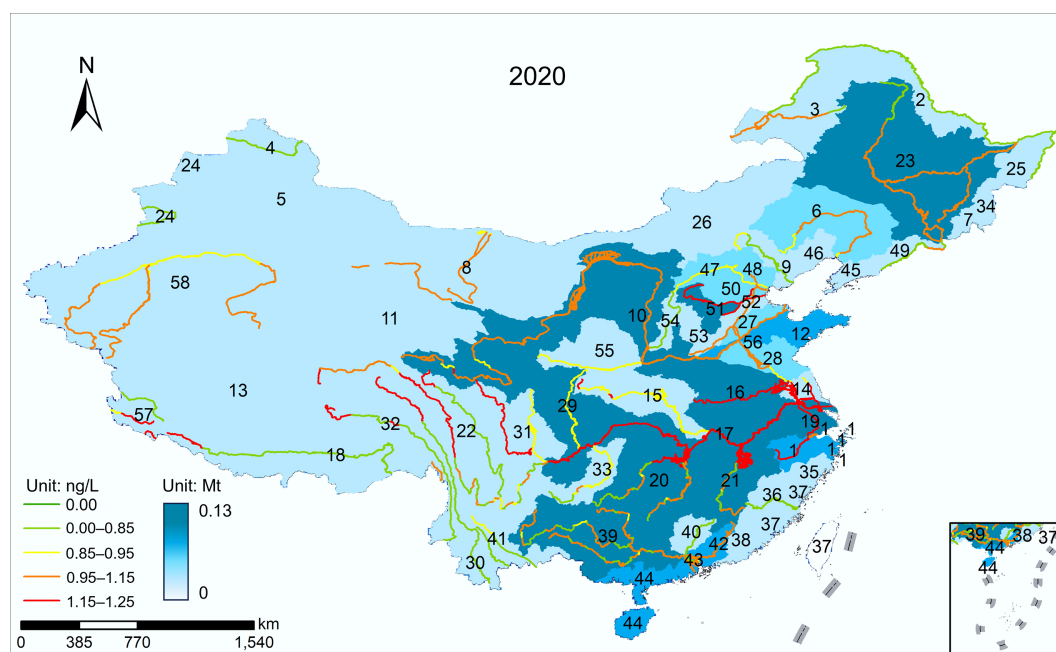


Fig. 3 The concentration distribution of 6PPD in China's secondary river basins in 2020. Note: This figure is based on the standard map service of the National Platform for Common GeoSpatial Information Services (<http://www.tianditu.gov.cn>), with the map approval number GS(2024)0650. The administrative boundaries remain unmodified.

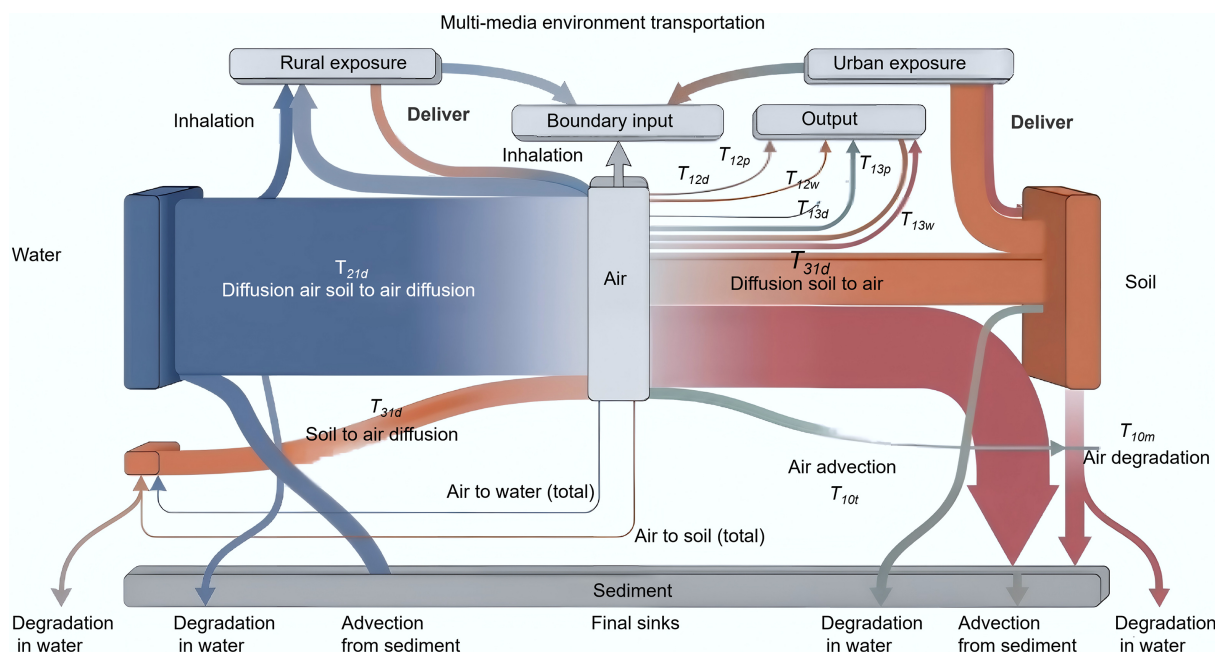


Fig. 4 Conceptual framework of 6PPD multimedia fate and transport in the coupled air-water-soil-sediment system. Arrows indicate dominant migration pathways (T_{21d} : water-to-air diffusion; T_{31d} : soil-to-air diffusion; T_{12d} : air to water diffusion; T_{12p} : air-to-water dry precipitate; T_{12w} : air-to-water wet precipitate; T_{13d} : air-to-soil diffusion; T_{13p} : air-to-soil dry precipitate; T_{13w} : air-to-soil wet precipitate; T_{10m} : air degradation; T_{10t} : air advection outflow). Minor processes (T_{12} , T_{13} series) are omitted for clarity. The width of arrows is proportional to flux magnitude.

watershed environments^[30]. Water-to-air (T_{21d}) and soil-to-air diffusion (T_{31d}) constitute the major inter-compartment exchange processes, indicating that volatilization and re-partitioning contribute to the continual cycling of 6PPD among environmental media.

The basin-level results in [Supplementary Tables S10 and S11](#) further confirm this pattern across China's 58 secondary river basins. Air degradation fluxes (T_{10m}) range from 6.99×10^2 to 1.30×10^3 mol/h with the highest values observed in the Poyang Lake basin (1.30×10^3 mol/h), Yangtze River basin (1.14×10^3 mol/h), and Huaihe (1.13×10^3 mol/h) basins, reflecting intensive emissions and active multimedia exchange in densely populated and highly urbanized regions. Water-to-air diffusion (T_{21d}) exhibits a similar magnitude, ranging from 6.79×10^2 to 1.28×10^3 mol/h, indicating that atmospheric degradation and water-air exchange together dominate the environmental transport of 6PPD. In most basins, T_{21d} and T_{10m} account for more than 98% of the total major transport fluxes, demonstrating a strong coupling between volatilization from aquatic systems and subsequent atmospheric degradation. By comparison, soil-to-air diffusion (T_{31d}) remains nearly constant at approximately 2.02×10^1 mol/h among basins, contributing only about 1–2% of these major fluxes. Other pathways, including air-to-water diffusion, air-to-soil diffusion, wet deposition, dry deposition, and atmospheric advection outflow, are negligible, mostly ranging from 10^{-25} to 10^{-7} mol/h. The spatial pattern of dominant fluxes generally corresponds with regions of intensive transportation activity and urban development, consistent with previous studies identifying traffic density and urbanization as key determinants of tire-derived contaminant emissions and redistribution^[47].

Together, [Fig. 4](#) demonstrates that the dominant migration pathway of 6PPD in China can be characterized as a "terrestrial accumulation-aquatic exchange-atmospheric degradation" process. Soil and road-adjacent environments act as important receiving reservoirs, while aquatic systems serve as active exchange compartments rather than passive sinks. The comparable magnitudes of T_{21d} and

T_{10m} indicate rapid cycling between water and air, followed by efficient atmospheric transformation, making atmospheric degradation the principal environmental removal mechanism. In contrast, the extremely low deposition and advection fluxes suggest limited contributions from direct atmospheric fallout and long-range atmospheric transport. These findings are consistent with previous studies showing that stormwater runoff and hydrological transport are the primary mechanisms by which tire-derived contaminants are transferred from road environments to receiving waters^[48]. Therefore, environmental control strategies should focus not only on reducing tire-derived emissions at the source, but also on interrupting runoff-mediated transport from roads and soils to aquatic systems. Such pathway-oriented management is particularly important because the transformation product 6PPD-quinone can be generated during environmental transport and has been identified as a major driver of aquatic toxicity and urban runoff mortality events^[29].

Future 6PPD emissions in China

The predictive reliability of the PCA-BP model was validated by comparing its projected 6PPD emissions against estimated emissions back-calculated from observed vehicle ownership over 2021–2024 ([Supplementary Table S12](#)). For the training-validation period (2021–2022), the model-predicted emissions agreed closely with estimated values, with relative errors of –0.51% and 1.93% and an overall MAPE of 1.22%. For 2024, the model projected a national 6PPD emission of $1.10\text{--}5.60 \times 10^{-2}$ Mt, which aligns well with the estimated emission of $1.11\text{--}5.10 \times 10^{-2}$ Mt, a deviation of 7.78–8.24%. This consistency confirms that the PCA-BP framework reliably captures the near-term drivers of emission growth and provides a credible basis for the long-term projections presented below.

The PCA-BP model projected continued increases in national 6PPD emissions over the 2021–2060 period under the SSP2 baseline ([Fig. 5](#)). Minimum and maximum national 6PPD emissions are

projected to reach $1.53\text{--}7.63 \times 10^{-2}$ Mt by 2030, $2.61\text{--}13.06 \times 10^{-2}$ Mt by 2050, and $2.93\text{--}14.64 \times 10^{-2}$ Mt by 2060, respectively, representing increases of 4.92–11.9 times, 20.1–20.4 times, and 22.5–22.9 times relative to the 2,000 baseline. The wide minimum–maximum range reflects the 0.4–2.0% uncertainty in the 6PPD mass fraction in tire rubber and the scenario-dependence of fleet growth.

The growth trajectory shows a deceleration after 2050: annual growth rates of 1.31–8.97% during 2021–2050 decline to 1.10–1.21% during 2051–2060. This reflects the anticipated plateau in per-capita vehicle ownership that typically accompanies economic maturity. However, even under slowing growth, the absolute emission level in 2060 remains substantially higher than in 2020, indicating that fleet electrification alone will not eliminate tire-derived chemical pollution. Electric and hybrid vehicles still use rubber tires and generate TWP through the same tire-on-pavement abrasion mechanism; higher vehicle mass in battery-electric vehicles may even increase per-kilometer tire wear compared with conventional vehicles of equivalent size.

These projections have direct relevance for long-range environmental planning. The secondary river basins currently identified as hotspots are expected to remain high-risk areas throughout the projection period, and new hotspots may emerge as urbanization expands into currently lower-emission western regions. Proactive installation of stormwater treatment infrastructure in growing cities can pre-emptively reduce future aquatic loads at lower cost than retrofitting established urban areas^[49].

Future perspectives and implications

This study developed a national-scale source-to-receptor framework for 6PPD in China by integrating city-level emission inventories, basin-scale multimedia fate modeling, and future scenario projections. The results reveal clear spatial heterogeneity in 6PPD emissions and environmental distribution, with rural roads representing the dominant emission source, eastern China exhibiting pronounced hotspots, and soil serving as a major long-term reservoir. Future projections further indicate that 6PPD emissions are likely to continue increasing through 2060 despite the rapid adoption of new energy vehicles, highlighting the growing importance of non-exhaust traffic emissions. Methodologically, the combination of high-resolution spatial allocation, multimedia fate modeling, and PCA-BP-based scenario prediction provides a transferable framework for assessing tire-derived contaminants at large spatial scales. Given the increasing

recognition of tire-derived chemicals as emerging contaminants in aquatic and terrestrial environments^[42,43], the framework can support future environmental monitoring, pollution control prioritization, and policy development in China, and can be readily adapted to other tire-related chemicals and rapidly motorizing regions worldwide.

Despite these advances, several uncertainties remain. The application of the IUCN allocation factors to 6PPD does not explicitly resolve particle-size-dependent transport behavior: larger TWPs ($>20\text{ }\mu\text{m}$) tend to deposit near roadways, while smaller particles may be resuspended or transported via stormwater runoff, resulting in spatially heterogeneous retention patterns that are not captured by the steady-state assumption. Surface retention in the road drainage system and leaching of 6PPD from the TWP matrix into the aqueous phase are also not accounted for in the current framework, which may result in an overestimation of soil loading rates and an underestimation of water-phase transport. The steady-state multimedia fate model does not capture short-term concentration peaks caused by stormwater runoff and sewer overflow events, which may generate episodic exposures far exceeding long-term average concentrations^[36,37]. Uncertainties associated with emission factors, environmental parameters, and future socioeconomic pathways may also influence model predictions. Future studies could improve the framework by incorporating transformation kinetics, event-based hydrological processes, and more extensive monitoring data from different environmental compartments. Nevertheless, both the emission inventory and modeled environmental concentrations were systematically validated against available observations, demonstrating good agreement with reported data. These validations provide confidence in the reliability of the framework and support the conclusion that the spatial patterns, future trends, and management implications identified in this study offer a robust scientific basis for understanding and mitigating tire-derived chemical pollution in China.

Conclusions

This study presents the first national-scale assessment of 6PPD emissions, environmental distribution, and multimedia fate associated with vehicle tire wear in China. By integrating a city-level emission inventory with basin-scale fate modeling, a source-to-receptor framework was established linking traffic activities to environmental exposure across 58 secondary river basins. National 6PPD emissions

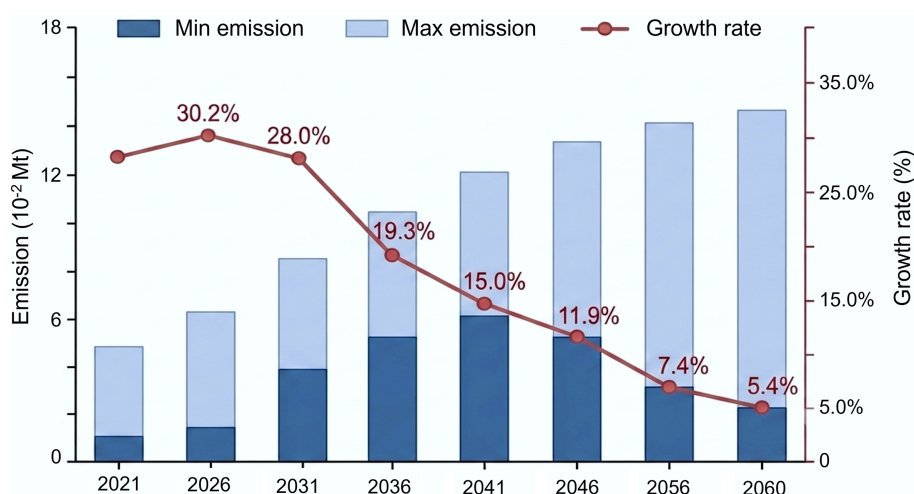


Fig. 5 Long-term emission projections and 5-year growth trends of 6PPD released from tire wear particles in China (2021–2060).

increased approximately seven-fold between 2000 and 2020, with rural roads representing the largest source category. Soil was identified as the primary receiving compartment, while modeled concentrations in rivers were consistent with available monitoring data. Multimedia transport analysis demonstrated that atmospheric degradation and water-air exchange are the dominant environmental processes governing 6PPD redistribution, whereas direct atmospheric deposition and long-range transport play minor roles. Future projections suggest continued growth of 6PPD emissions through 2060 despite ongoing vehicle electrification, indicating that non-exhaust traffic emissions will remain an important source of environmental contamination. These findings highlight the importance of managing runoff-mediated transport pathways in addition to controlling emissions at the source. The framework developed here provides a foundation for future assessments of 6PPD and supports the development of science-based strategies to mitigate tire-derived pollution in rapidly urbanizing regions.

Supplementary information

It accompanies this paper at: <https://doi.org/10.66178/aie-0026-0016>. A detailed description of the model framework and parameters, tables of modelling data, and additional figures.

Author contributions

The authors confirm their contributions to the paper as follows: Guang-Guo Ying and Qian-Qian Zhang designed the project; Wentao Teng performed the model simulations, analyzed the emission projection data, and prepared the figures; Xiaoyi Yu, Yaya Cai and Jian-Liang Zhao contributed to data curation, validation, and the interpretation of growth trends; Guang-Guo Ying, Qian-Qian Zhang and Wentao Teng drafted and revised the manuscript. All authors reviewed and approved the final version of the manuscript.

Data availability

Data will be made available on request.

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Competing interests

The authors declare that they have no conflict of interest.

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