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Document Version

Final published version

Citation (APA)

Ye, C., Jiang, F., Wang, F., Kapelan, Z., Xu, Z., Templeton, M. R., & Chu, W. (2025). Identification, sources and accumulation behavior of priority odorants discharged to surface water from stormwater systems with illicit connections. *Water Research*, 287, Article 124313. <https://doi.org/10.1016/j.watres.2025.124313>

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Identification, sources and accumulation behavior of priority odorants discharged to surface water from stormwater systems with illicit connections

Cheng Ye^{a,b,c,1}, Fangyuan Jiang^{a,b,c,1}, Feifei Wang^d , Zoran Kapelan^e,
Zuxin Xu^{a,b,c}, Michael R. Templeton^f , Wenhai Chu^{a,b,c,*} 

^a State Key Laboratory of Water Pollution Control and Green Resource Recycling, College of Environmental Science and Engineering, Tongji University, Shanghai 200092, China

^b Ministry of Education Key Laboratory of Yangtze River Water Environment, Tongji University, Shanghai 200092, China

^c Shanghai Institute of Pollution Control and Ecological Security, Shanghai 200092, China

^d School of Environmental and Chemical Engineering, Shanghai University, Shanghai 200444, China

^e Delft University of Technology, Department of Water Management, Stevinweg 1, 2628CN Delft, the Netherlands

^f Department of Civil and Environmental Engineering, Imperial College London, London, SW7 2AZ, United Kingdom

ARTICLE INFO

Keywords:

Odorants
Quantitative structure-property relationship
Rainfall events
Sewer sediment
Storm sewer

ABSTRACT

The odor nuisance of urban surface water after rainfall events has aroused public concerns and threaten the aquatic organisms. Herein, the first study to investigate 150 odorants in storm sewer discharge was performed in humid regions of China. During rainfall events, the total concentrations of odorants at storm sewer outlet increased by 1.3–2.1 fold from 1.7–9.4 µg/L to 2.1–20.0 µg/L with 37 odorants having detection frequencies above 50 % on rainy days, and the concentrations of total odorants in air also significantly increased resulting in worse odor nuisance. The accumulation of odorants in sewer sediment and the remobilization of sewer sediment were factors resulting in more intensified emission of odorants from storm sewer on rainy days. More than half of odorants discharged during rainfall were contributed by sewer sediment. Thioethers, indoles, 2-isopropyl-3-methoxy pyrazine, acetophenone and coumarin exhibited high sediment-accumulation. Quantitative structure-property relationship models revealed that enhanced sediment-accumulation of chained aliphatic and aromatic odorants can be explained by the electrostatic attraction and topological characteristic, respectively. The multicriteria analysis was further introduced for relative odorants ranking by considering the variations in hazard criteria of environmental occurrence, ecotoxicity, persistence, odor nuisance and sediment accumulation. Among priority odorants, thioethers and indoles were attributed by their distinct sediment-accumulation and odor nuisance potential, while chlorinated anisole and pinenes prioritized due to their higher ecotoxicity. These findings provide novel insights into the odorants from storm sewer discharges and explore the environmental behaviors of odorants in sewer sediment.

1. Introduction

Rainfall events in the urban environment have increasingly become an environmental concern due to their significant impact on surface water quality (Lapointe et al., 2022; Sinha et al., 2017). During these events, various contaminants, including toxic, non-biodegradable and emerging pollutants, are extensively released into surface waters via

different urban wet weather flows including urban runoff, combined sewer overflow and separate sewer overflow, posing acute toxicity risks to aquatic organisms and chronic health risks to humans through drinking water exposure (Tian et al., 2021). Notably, due to the dominance of separate storm sewer in the urban areas of China, whose length are 5.5 times that of combined sewer, the storm sewer discharge exhibited higher environmental risks. In humid regions of China, which

* Corresponding author at: Room 407, National Engineering Research Center for Urban Pollution Control, 1239 Siping Road, Yangpu District, Shanghai, 200092, China.

E-mail address: feedwater@126.com (W. Chu).

¹ Cheng Ye and Fangyuan Jiang contributed equally to this work.

<https://doi.org/10.1016/j.watres.2025.124313>

Received 12 May 2025; Received in revised form 2 July 2025; Accepted 27 July 2025

Available online 29 July 2025

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was the investigated area of this study, concentrations of micro-pollutants in storm sewer outlets have been reported to range from 490 to 1659 ng/L, with discharge loads exceeding those of treated wastewater effluent by a factor of 2.4 (Yang et al., 2025).

One distinct characteristic of water quality deterioration after a rainfall event caused by storm sewer discharge is the odor pollution of natural waterbodies (Bin et al., 2019). Potential health concerns, such as asthma, atopic dermatitis and neurologic damage, can result from long-term exposure to varieties of odorants (Byliński et al., 2019; Piccardo et al., 2022; Zheng et al., 2020). Nevertheless, little information is currently available on the odorants in storm sewer discharge during rainfall. Hydrogen sulfides, methyl mercaptan and sulfides were identified to be significant contributors to sewer escaping odors in Australia (Sivret et al., 2016; Liang et al., 2019). However, compared with the air pollution caused by inorganic odorants with high volatility, the organic odorants discharge from storm sewers exhibited higher potentials in threatening water quality and human health due to their persistence and toxicity besides odor nuisance (Namour, 2022). It underscores the necessity of a comprehensive investigation into the odorants in storm sewer with increased urbanization and climate change (Rubinato et al., 2024).

Diverse sources can contribute odorant loads to storm sewer discharges during rainfall events. Motor vehicle emissions and widespread usage of different paints and plasticizers have contributed substantial volatile organic compounds in urban environments including alkanes, alkenes, aromatic hydrocarbons and halogenated hydrocarbons, which can be flushed out by stormwater (Huang et al., 2021; Sivret et al., 2016). Furthermore, the widespread illicit connection (i.e., either internation and accidental connections of wastewater directly into storm sewers) can result in the wastewater-related odorant discharge into surface water via storm sewers (Du et al., 2020; Xu et al., 2019). It was found that approximately 38 % untreated wastewater was illicitly connected into storm sewer in China (Xu and Xu, 2022). The wastewater-related odorants (e.g., pyrazines, *p(m)*-cresol, benzaldehyde and so on) were frequently detected in rivers of China (Wang et al., 2021). In addition, sewer sediments are critical to the occurrences of odorants. During dry weather, under the input of wastewater, the odorants may be accumulated or depleted in sewer sediment via complex reactions. For example, some benzene-derivative odorants (e.g., 1, 3-xylene, 1,4-xylene and 1,2-xylene) can be adsorbed into sewer sediment attributed to their relatively higher level of hydrophobicity (log K_{ow} , 2.9–4.2) (Hua et al., 2022). Meanwhile, xylene also can be decomposed by sediment microorganism under anaerobic or aerobic conditions (Su et al., 2022). During wet weather, the remobilized sewer sediment can be an important odorant source under the flushing of urban runoff. However, compared to the sediments in sewage systems, significant gaps remain in understanding of the occurrence, sources and environmental behaviors of odorants in sediment of storm sewer with illicit connection.

The environmental behaviors of organic compounds with similar structures can be effectively revealed by quantitative structure–property relationship (QSPR) models from their physicochemical, quantum-chemical and topological properties (Huang et al., 2021; Stults et al., 2023). Zhang et al. (2024) disclosed the key molecular parameters influencing the bioaccumulation potential of 25 organophosphate esters using QSPR models. However, the accumulated or depleted behavior of organics in sewer sediment have been barely investigated using QSPR models. Previous studies using QSPR models only focus on the sediment or soil sorption property of organics regardless of biotransformation role (Kahn et al., 2004; Tang et al., 2024), which may be inappropriate for predicting environmental behaviors of organic in sewer sediment undergoing complicated biological reactions. At the same time, given the complex mixtures of odorants from storm sewer discharge to aquatic environment, it is necessary to identify the priority odorants that serve as primary risk drivers to facilitate pollution control strategies. Identifying priority contaminants has been investigated in recent years (Wei

et al., 2024), but comprehensive identification methods for odorants discharged from storm sewer have not yet been established incorporating occurrence levels, odor nuisance, ecological toxicity, persistence and sediment-accumulation potential (Ruan et al., 2023).

Therefore, the specific objectives of this study were 1) to comprehensively investigate the composition and concentrations of odorants discharged from storm sewer, 2) to evaluate the environmental behaviors of odorants in sewer sediment, 3) to explore the accumulation or depletion behaviors of odorants with different chemical structures in sediment and 4) to identify the priority odorants discharged from storm sewers. The overall aim of the study was to further improve the understanding of pollutants with respect to urban storm sewer and support the development of regulations for the pollutant management during rainfall events.

2. Materials and methods

2.1. Study areas

We selected the separate storm system of the built-up urban area to determine the characteristics of odorants discharged from storm sewer in three cities (Figure S1). The selected cities are located in humid regions of Southern China (30°01′–32°43′N, 118°31′–121°31′E) with annual average rainfall of about 1200–1500 mm, representing typical mid-latitude humid urban areas in China. For city A and C, the separate storm systems were retrofitted from previous combined sewer systems, with some sanitary sewage still illicitly connecting into the separate storm system. For city B, the separate storm system was laid prior to construction of buildings, and some individual units illicitly connected sanitary sewers into the separate storm sewer. After careful investigation, the illicit connection points were confirmed. In order to ensure that the untreated wastewater was not directly discharged into the receiving water in on sunny days, intercepted sewers were set up along the river in three cities, which was as the location of the storm sewer outfall sampling point. Specific information on the selected storm sewer in three cities was provided in Table S1.

2.2. Sampling collection

Odorants discharged from storm sewer and in air nearby storm sewer outlet were monitored in three storm sewer outlets. The detailed information on each sampling rain event is provide in Table S2. In order to reflect the effect of rainfall on odorants discharged from storm sewer, the occurrence of odorants in the baseflow (mainly composited of illicitly-connected wastewater) of storm sewer on sunny days were also investigated. Hence, the sampling campaign was conducted involving 28 sunny and 22 rainy days (minimum daily precipitation higher than 1 mm to ensure the formation of urban runoff). On rainy days, water samples at outlets were collected 30 min after the start of rainfall event, when the flow in sewer can reach 0.5 L/s even in the rainfall of 1 mm, to ensure sufficient water sampling volume. Water samples from runoff and effluent were then collected every 30 min of the first hour, and every hour thereafter until runoff and rainfall ended. Moreover, the air sample was simultaneously collected at 0.5 m above the outflow above the storm sewer using PTFE air collecting bag.

The overlaying water and sediment samples of illicit connection points in storm sewer were collected at relevant manholes three times during sunny days, taking 1 L of overlaying water samples at 10 cm below top water surface and 1 kg of sediment samples at 20 cm below bottom water surface. We collected the water and sediment samples using stainless-steel bucket/grabber and samples were collected into a glass container without headspace. As for runoff sampling in nearby surface of storm sewer (R1–R4 points in Figure S1), it was conducted at the 30 min after rainfall with volume of 1 L. After sampling, 1 mL of 0.1 mol/L ascorbic acid solution was added to reduce the oxidation of odorants. Then, the samples were immediately transformed into

laboratory and stored at 4 °C, with analysis completed within 48 h.

2.3. Analytical methods and data analytics

The detailed information about chemicals and reagents used in this study can be seen in Text S1. The odorants in collected overlaying water and sediments were enriched by means of headspace solid-phase microextraction (HS-SPME) method according to previous study (Wang et al., 2019). Further details about the HS-SPME are provided in Text S2. Detailed information on instrumental parameters used in odorant analyses and for the quality assurance and quality control are provided in Text S3 and Text S4, respectively. Total 150 odorants, which were frequently detected in surface water, wastewater and drinking water, were determined. Detected odorants were divided into 12 groups according to their basic chemical structure, including alcohols (Alc), aldehydes (Ald), non-oxygen benzene-containing compounds (Bez), esters (Est), ethers (Eth), indoles (Ind), ketones (Ket), phenols (Phol), pyrazines and pyridines (Pyr), terpenes and terpenoids (Terp), thioethers (Thio), volatile fatty acids (Vfa). Detailed odorant concentrations were collected in Table S5 and S6. Detailed information and analysis methods of basic water quality parameters are described in Text S5.

Furthermore, the sediment accumulation factor (SAF) index was calculated to evaluate the accumulation behavior of odorant in sediment:

$$C_{\text{sediment-TOC}} = C_{\text{sediment}} / \text{TOC}_{\text{sediment}} \quad (1)$$

$$\text{SAF} = C_{\text{sediment-TOC}} / C_{\text{water}} \quad (2)$$

where C_{sediment} (ng/g) and $\text{TOC}_{\text{sediment}}$ (%) are the concentration of each odorant in sediment and the total organic carbon concentration of sediment, respectively. $C_{\text{sediment-TOC}}$ (L/g) is the lipid-normalized concentration of each odorant. Spearman rank correlation analysis and redundancy analysis required for the analysis of environmental factors and source identification were performed by IBM SPSS Statistics 26.

2.4. QSPR modelling

The detected odorants were divided into chained aliphatic, cyclic aliphatic and aromatic odorants for QSPR modeling. The octanol-water partition coefficient (K_{ow}), the quantum chemical descriptors and eight topological descriptors were adopted to develop the QSPR models. Among these descriptors, the octanol-water partition coefficient was obtained from the EPI Suite (version 4.1), and the topological descriptors were calculated using Rdkit package of Python (version 3.10). The quantum chemical descriptors were obtained calculated using Gaussian 09 W software using B3LYP/6-31g(d) and B3LYP/DEF2TZVP basis (Li et al., 2022) and detailed descriptors were analyzed by Multiwfn program (Lu and Chen, 2011). The dataset of each type of odorant were randomly divided into training and validation sets using a 4:1 ratio (i.e. 80 % data was used for training and 20 % for validation). The QSPR model of odorants revealing the connections between SAF and descriptors was developed using a Multi-linear Regression model implemented using the Scikit-learning package in Python (version 3.10) (Gao et al., 2021). For internal validation, the bootstrap method correlation coefficient (Q_{BOOT}^2) was applied to evaluate the robustness of the developed models. For external validation, the external explained variance (Q_{EXT}^2) and external determination coefficient (R_{EXT}^2) were calculated based on the external test set to evaluate the predictive capability of the models. The detailed values of descriptors are presented in the Supplementary Data spreadsheet.

2.5. Priority odorant identification

Previous studies usually identified the key or priority odorants based solely on the odor active value or detection frequency (Agus et al., 2011;

Zhao et al., 2024). In our study, a modified methodology was established incorporating five criteria, including occurrence, ecotoxicity, persistence, sediment accumulation and odor nuisance to identify the priority odorants. The total score for each odorant was obtained by summing the five criteria values with equal weight factor. Subsequently, the target compounds were categorized into five classes (I-V) by geometric progression (Wang et al., 2023), and the odorants identified as Class I were deemed as priority odorants from storm sewer discharge. Further details can be found in Text S6.

3. Results and discussion

3.1. Intensified odorant emission from storm sewer during rainfall

The odorant concentration in base flow of storm sewers on sunny days and effluents of storm sewers at different rainfall intensities are presented in Fig. 1a. On dry days, the odorant concentration of base flow of storm sewers showed that city C (4030.0 ± 600.4 ng/L) > city B (2733.1 ± 597.5 ng/L) > city A ($2052.3.0 \pm 1239.4$ ng/L), which may be attributed to the higher population density (4036.45 people/km²) and illicit connection ratio (20 %) of storm sewer in city C (Table S1). For odorant composition, indoles and thioethers are dominate odorants in the base flow with average proportion accounting for 50.4 %–60.6 % of the odorants in the based flow (Fig. 1b-d). The average concentration levels of terpenes and terpenoids, pyrazines/pyridines and phenols exhibited regional differences. The average concentrations of terpenes and terpenoids, pyrazines/pyridines and phenols in base flow of city C were 1.9–4.1, 16.2–21.3 and 2.2–2.6 times higher than those in city A and B. This difference may be attributed to the fact that the service area of storm sewer in city C is relatively functionally diverse (Figure S1). Terpenes and terpenoids, pyrazines/pyridines and phenols are often used as flavor-adding agents, bleaches, softener and other chemicals widely applied in commercial and administrative area (Luo et al., 2025). Overall, there was no significant difference in the odorant composition in different storm sewers.

Notably, the average odorant concentrations of city A, B and C during rainfall were 2798.1 - 3555.7, 3634.0 - 5675.2 and 5591.6 - 12,283.5 ng/L, respectively. The average odorant concentration of storm sewer effluent during rainfall were 1.3–3.0 times that of base flow during dry weather. In addition to concentration elevation, 16 odorants (e.g., tetramethylbenzene, ethyl acetate, 2-chlorophenol, 2,6-di-tert-butyl-4-methylphenol, propanoic acid) were additionally detected among the 57 odorants detected on rainy days, and 36 odorants can be detected with frequencies above 50 % (Figure S2). When the urban runoff enters the storm sewer, tow simultaneous effects occur. Firstly, the odorants, such as volatile organic compounds escape from architectural coating (e.g., methylbenzene and butyric acid) and oil fuel (e.g., ketones and esters) can be carried into storm sewer via wet precipitation and road flushing (Müller et al., 2020). Elevated concentrations of such odorants were particularly pronounced in the storm sewer of city C with higher urbanized degree. The average concentrations of benzene-derivatives, esters, and ketones during light rainfall increased by 4.7, 9.3 and 6.1 times compared to those during dry weather (Fig. 1d). By comparison, the average concentrations of benzene-derivatives, esters, and ketones in city A and B achieved highest levels during moderate rainfall, which may be attributed to lower density of road traffic and buildings. Simultaneously, the sewer sediment will be remobilized under the flushing of urban runoff. The odorants in sewer sediment of investigated storm sewer showed that city C (6564 ± 483 ng/g) > city B (3851 ± 456 ng/g) > city A (1306 ± 364 ng/g) (Fig. S3). The significant increases of odorants in the discharge from storm sewer of city C during rainfall can be explained by the higher content of odorants in sewer sediment of city C. However, when the rainfall reaches a certain level, the increase in flushing effect was comparatively small in relation to the magnitude of rain dilution, therefore the odorant concentrations decreased during heavy rainfall.

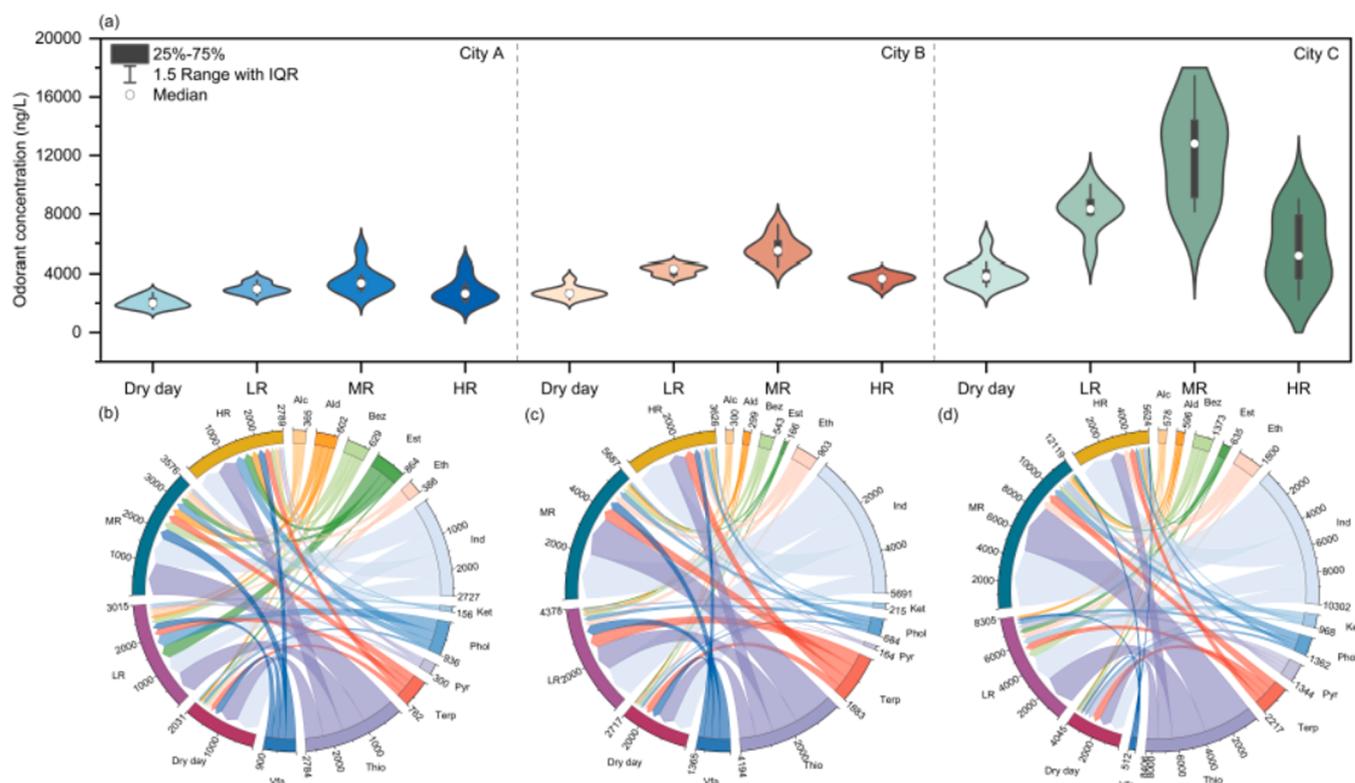


Fig. 1. The concentrations and profiles of odorants in investigated storm sewers during dry days and at different rainfall intensities.

The discharges from storm sewers contributed considerable odorants to surface water on sunny days according to the concentrations of odorants at a storm sewer outlet. For instance, the average concentrations of 1,4-xylene (Bez4), indole (Ind1) and dimethyl trisulfide (Thio3) were only found to be 4.9, 14.7 and 2.1 ng/L in raw water across China (Wang et al., 2021), respectively. However, the average concentrations of these at storm sewer outlet on sunny days were 28.0, 35.0 and 98.1 times higher than those in surface water, respectively. As shown in Fig. S4, the odorant in air nearby storm sewer outlets were found to significantly increase after rainfall. Moreover, 14 odorants (with star labels in Fig. S4), with higher saturated vapor pressure (above 800 Pa under 20 °C), were additionally detected in the air nearby to the storm sewer. Clearly, the rainfall can amplify the emission of odorants from storm sewers, and tends to be higher during moderate rainfall.

3.2. Sources of odorants in storm sewer during rainfall events

Anthropogenic (i.e., illicitly-connected wastewater) and natural (urban runoff) factors within the service area of storm sewer were considered as the contributors to the odorant in storm sewer. Correlation analysis was adopted to reflect the disparities in odorant source and emission patterns. Positive correlations can be observed between most detected odorants at storm sewer outlet on sunny days (Figure S5) such as phenol (Phol7) and 4-methylphenol (Phol11) ($r = 0.40$, $P = 0.03$), 2-isopropyl-3-methoxy pyrazine (Pyr6) and 1,4-dichlorobenzene (Bez 9) ($r = 0.47$, $P = 0.04$). Almost odorants on sunny days were widely used raw materials or additives in antioxidant, essence, plasticizer and other daily chemical products, which can be carried by domestic and industrial wastewater (Culleré et al., 2009; Weston-Green et al., 2021; Yu et al., 2013). It can be inferred that the illicitly-connected wastewater dominated the odorants of storm sewer on sunny days from the positive correlations between the base flow and illicitly-connected wastewater (Table S7). The concentrations of odorants in illicitly-connected wastewater sewers and urban runoff near three storm sewer outlets are shown in Figure S6. As it can be seen from this figure, the

illicitly-connected wastewater introduces substantial amounts of odorants (1.5–3.9 $\mu\text{g/L}$) to the flow in storm sewer, causing a higher content of odorants in storm sewer outlet on sunny days.

With respect to the discharge of storm sewer on rainy days, the concentrations of odorants were relatively lower in urban runoff near the storm sewer outlets (1.0–3.3 $\mu\text{g/L}$), which was supposed to dilute the discharge of odorants from storm sewer instead of increasing concentrations on rainy days. Furthermore, only weak correlations ($r < 0.3$, $p < 0.05$) can be found in the cumulative concentrations of urban runoff in terms of alcohols, aldehydes, benzene derivatives. It highlighted that higher concentrations of odorant discharge from storm sewer on rainy days may be due to new odorant source of entering the storm sewer.

In the PCA analysis of Fig. 2a, some samples on rainy days were apparently separated from other sample cluster of the same city ($P < 0.05$ denoted by an asterisk), indicating that the conveyance of complex contaminant mixtures in illicitly-connected storm sewer might trigger the composition change of odorants during rainfall. The increased concentrations and changed composition of odorant highlighted the potential role of sewer sediment in odorants discharged from storm sewer during rainfall events in addition to illicitly-connected wastewater and urban runoff. Sewer sediment, as an accumulation of solid particulate matter and organic pollutant, is resistant to shear for rainfall washout and is prone to release a large number of suspended particles upon remobilization (Ahyerre et al., 2000). To confirm this conjecture, the redundancy analysis was performed to investigate the environmental factor affecting the odorants at storm sewer during rainfall (Fig. 2b). It revealed that TOC, SS and rainfall intensity (RI) were strongly related with the occurrence of odorants ($P < 0.05$, Table S8 and S9), which further demonstrated that rainfall-driven resuspension of sewer sediment intensified the odorants discharge from storm sewer during rainfall.

Furthermore, the mass contribution of different sources of odorants during different rainfall events were calculated, as described in Text S7. As shown in Figure S7, the mean contribution of odorants to storm sewer discharge during rainfall from illicitly-connected wastewater only

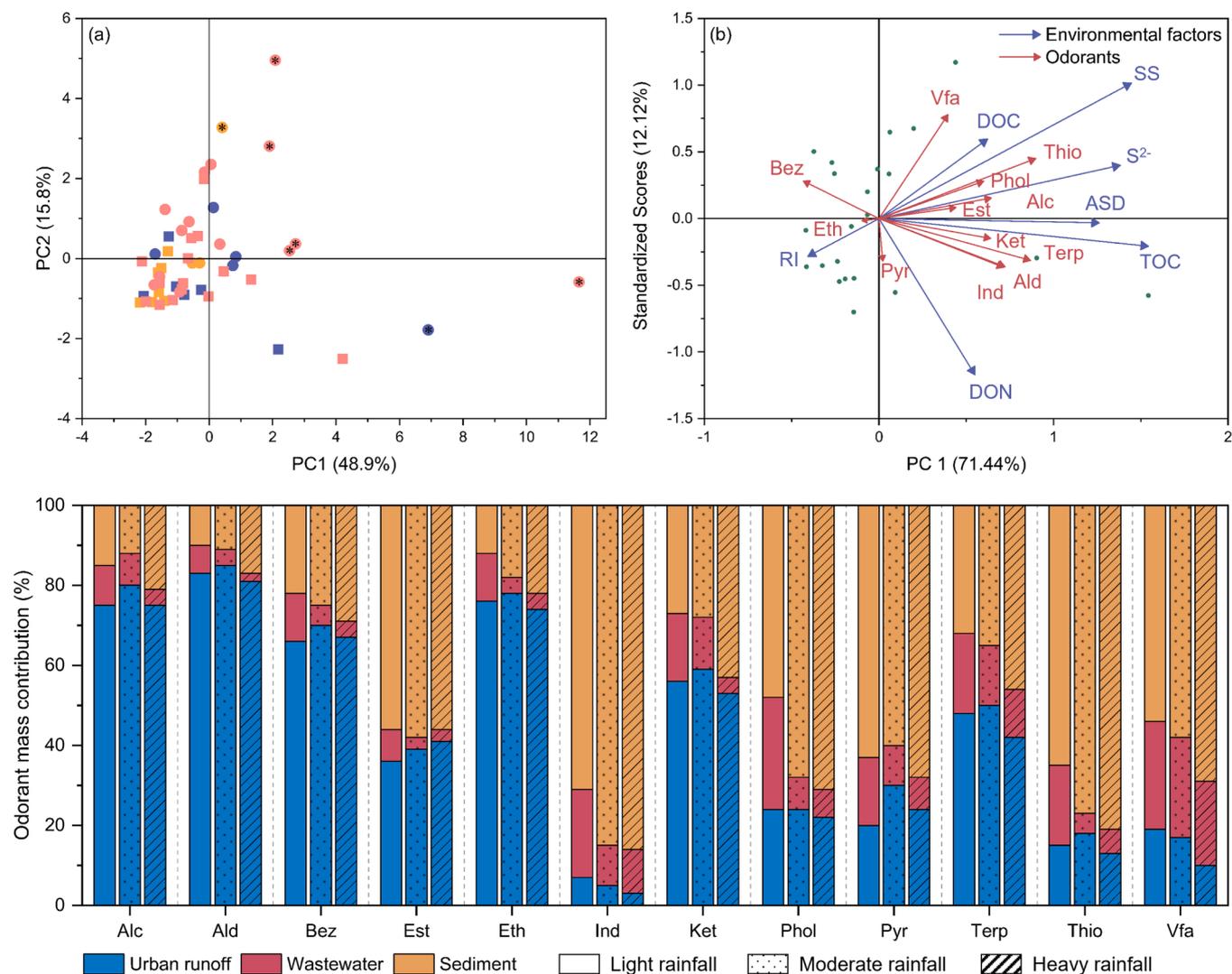


Fig. 2. The correlations between odorant concentrations and environmental factors, and sources apportionment for different odorant analogues. (a) Principal components analysis (PCA) analysis based on the odorants at storm sewer outlet. The squares represent samples collected on sunny days and the dots represent samples collected on rainy days (samples marked with an asterisk indicate significant deviations from the cluster, $P < 0.05$). (b) Redundancy analysis (RDA) of odorant concentration and environmental factors, (c) the odorant mass contribution of stormwater, wastewater and sediments from storm sewer discharge at different rainfall intensities.

accounted for 3.8 %–11.4 %. By comparison, the mobilized sediments contribute relatively higher proportion of odorant (42.5 %–78.6 %) to storm sewer discharge, and the contribution achieved highest percentages during moderate rainfall. Such changes were mainly due to the increased flushing effect of sediment and dilution effect of urban runoff with the increasing intensities of rainfall. In addition, the main source of odorants from storm sewer discharge during rainfall shows variations between different types of odorants (Fig. 2c). The contribution of odorants including alcohols, aldehydes, benzene derivatives, ethers, ketones and terpenes/terpenoids in storm sewer outlets from urban runoff ranged from 42 % to 85 %, indicating that the urban runoff is the primary source for these odorants in the discharge of storm sewer. Above urban runoff-dominated odorants were reported to be the main volatile organic compounds derived from transportation, industrial processes, solvent utilization and other purposes in urban areas, which can be easily flushed by urban runoff (Richardot et al., 2023; Wu and Xie, 2017). Other odorants from storm sewer discharge, including esters (56 %–58 %), indoles (71 %–86 %), phenols (48 %–71 %), thioethers (65 %–81 %) and volatile fatty acids (54 %–69 %), were mainly contributed by the mobilized sediments flushed by stormwater. The positive correlations between phenols, thioethers and indoles and antecedent

sunny days before rainfall were firstly observed among these sediment-contributed odorants (Fig. 2b). It suggested the more intensive odorant discharged from storm sewer on rainy days, were influenced not only by the rainfall events but also by the environmental behaviors of odorants in sewer sediment arising from illicitly-connected wastewater input on dry days.

3.3. Accumulated or depleted behaviors of odorants in sewer sediment

3.3.1. The variation of odorants in sewer sediment

Considering the potential contribution of sewer sediment to storm sewer discharge, the odorant concentration in sediments and SAFs were also determined to understand the fate of odorants in sediments during continuous sunny days. As shown in Fig. 3a, the concentrations of detected odorants in sediments showed different tendencies as sunny days continued to occur in sequence. Typically, the concentrations of indoles, thioethers and volatile fatty acids in sediments on 6th day increased by 52 %–4688 % compared to those on 1st day. By comparison, among the esters, ethers, terpenes/terpenoids and phenol-derivates, the concentrations of them in sediment continued to decrease over 6 days or increased then decreased. As shown in Fig. 3b,

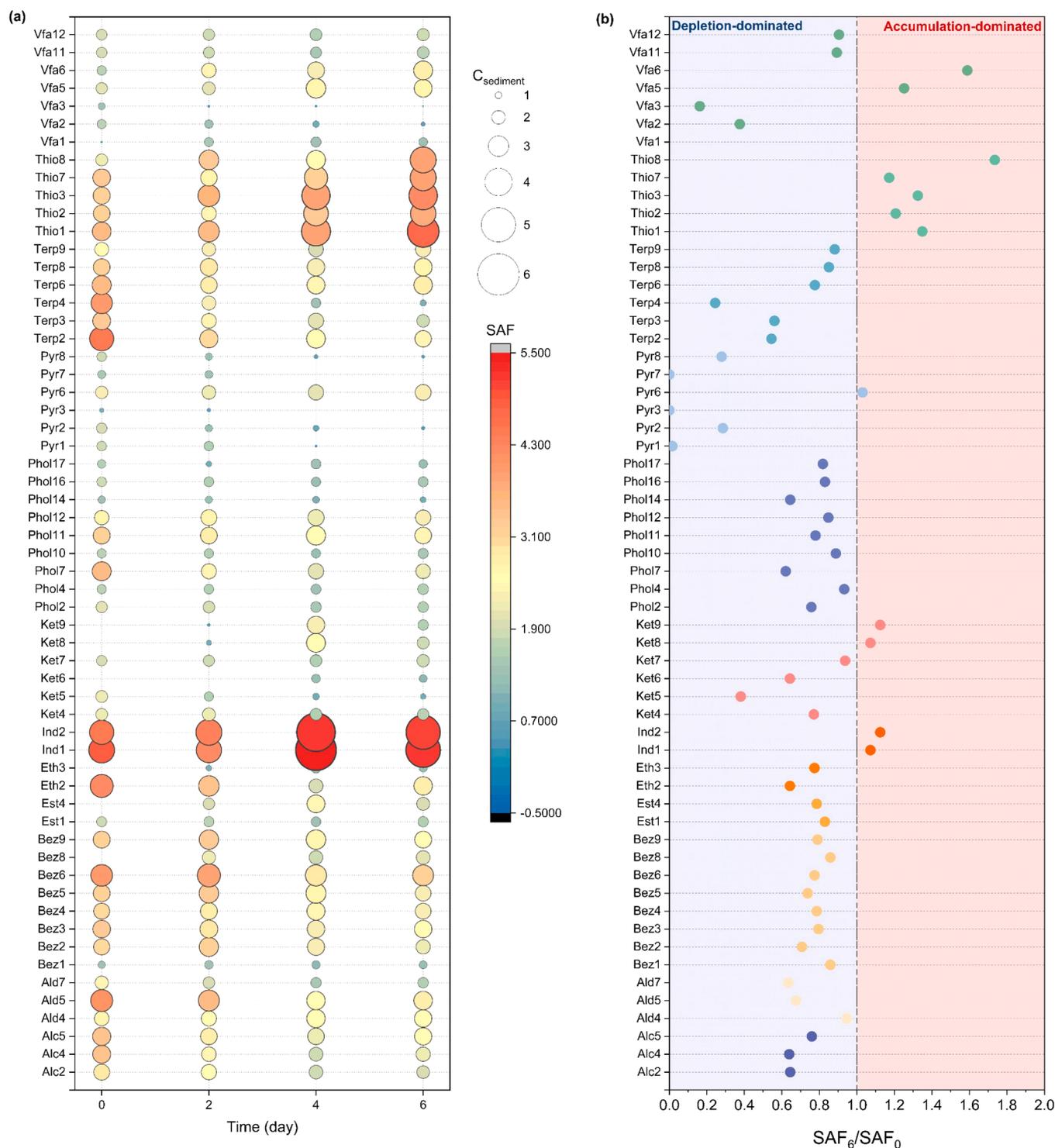


Fig. 3. The occurrence and variation of odorants in storm sewer sediment during continuous sunny days. (a) Concentrations and SAF of each odorant in sediment during continuous sunny days; (b) The ratio of each odorant's SAF on 6th day to that on initial day.

the ratio of each odorant's SAF on 6th day to that on initial day was further calculated to observe the dominated environmental behaviors (i. e., depletion or accumulation) of each odorant.

Thioethers and indoles exhibited significant potential to accumulate in storm sewer sediments with $\text{SAF}_6/\text{SAF}_0$ above 1.0, indicating that the mass of thioethers and indoles in per mass of sediment can continue to increase at least within 6 days. As for alcohols, aldehydes, benzene-derivatives and phenol- derivatives, they were significantly decreasing with the prolong of sunny days with the $\log\text{SAF}_6/\text{SAF}_0$ lower than 0.9.

This explained the significant accumulated potential of the indoles, thioethers and volatile fatty acids in sewer sediment.

Notably, some odorants were detected in the sediments but not in the illicitly-connected wastewater in a storm sewer (e.g., 2-methylpyrazine (Pyr1) and propanoic acid (Vfa2)). This can be attributed to two aspects. Firstly, since first sampling was conducted after a rainfall event (i.e., day 0), some odorants were carried in the stormwater but not in the illicitly-connected wastewater maybe remained in the sediments. Then, in the environment with relatively abundant oxygen level during initial sunny

days without stormwater input, the elevated levels of microbial community may facilitate the degradation stormwater-sourced odorants contributing to their continued decreasing tendencies in sewer sediment. For example, *pseudomonas*, which was found to be ubiquitous in wastewater sewer, can utilize the phenol and phenolic derivatives as carbon sources, typically chlorine-substituted derivatives like *o*-, *m*-, *p*-chlorophenol (Krastanov et al., 2013; Shi et al., 2023). Additionally, some odorants were originally produced from sediment such as volatile fatty acids. Jin et al. (2015) found that the microbial communities in biofilms would consume the organic macromolecules to produce volatile fatty acids (Jin et al., 2015).

In order to identify the dynamic changes of odorants in sewer sediment under the exogenous input (i.e., illicitly-connected wastewater), the correlation between K_{ow} and SAF was further investigated (Figure S8). The K_{ow} is commonly used as a hydrophobicity parameter, which reflects the affinity of organic pollutants to soil, sediment and aquatic organisms, and it has been used as a key indicator of biological utilization efficiency (Wagner et al., 2019). As shown in Figure S8a and b, strong correlation was found between log SAF and log K_{ow} for odorants on 1st ($r = 0.23$ and $P < 0.01$) and 2nd day ($r = 0.32$ and $P < 0.05$). This indicates that physical adsorption dominates the occurrence of odorants in storm sewer sediment in the initial few days after a rainfall event, where highly hydrophobic odorants preferred to adsorb on the sediment. For instance, the benzene derivatives (log K_{ow} of 2.54–4.18), ethers (log K_{ow} of 3.36–4.01) and terpenes/terpenoids (log K_{ow} of 2.85–4.83) with higher hydrophobic characteristics exhibited higher average log SAF of 0.53, 1.21 and 1.12 on first sampling day, respectively. With the prolonged period of sunny days, the positive correlations between log SAF and log K_{ow} gradually disappeared (Figure S8c and d). This suggests that the occurrence of odorants in sewer sediment is influenced by the combined effect in the physical adsorption and biotransformation, and the biological processes dominated the transformation of odorants after reaching the adsorption equilibrium between odorants and sediments as sunny days continued to occur in sequence.

3.3.2. QSPR models of SAF for the odorants

To better understand the environmental behaviors of odorants in sediment influenced by both biological metabolism and physical adsorption, QSPR models were established based on the SAF value. Considering that the similar environmental behaviors can be more easily found in the odorants with similar chemical structure, the detected odorants were categorized into three groups of chained aliphatic, cyclic aliphatic and aromatic odorants. The obtained QSPR models were as follows:

3.3.2.1. Chained aliphatic odorant

$$\text{SAF} = 0.19E_{HOMO} - 0.06\eta + 0.92V_{s,\min} + 0.20 + 2.22 \quad (3)$$

3.3.2.2. Cyclic aliphatic odorant

$$\text{SAF} = -0.02E_{LUMO} + 0.05V + 0.99\mu + 1.55 \quad (4)$$

3.3.2.3. Aromatic odorant

$$\text{SAF} = 0.45\mu + 0.78\text{Windx} + 0.34\text{ShpA} - 0.02\text{SVDe} + 2.13 \quad (5)$$

Table S10 shows the statistical performance of these models. As it can be seen from this table, all three models have good prediction performance as their R^2 values are above 0.60 and RMSE values are below 0.30. The higher Q_{BOOT}^2 (all >0.7), and R_{EXT}^2 as well as Q_{EXT}^2 (both >0.6) indicate the satisfactory robustness and prediction ability of the models. Moreover, no collinearity can be observed in all models, as demonstrated via VIF factors of all selected descriptors being all below 10 and the corresponding P values all being lower than 0.05.

As shown in Eq. (3), the positive fitted coefficient values were obtained for $V_{s,\min}$ (0.92) and E_{HOMO} (0.19) of the QSPR model for chained

aliphatic odorant (Table 1), reflecting the critical role of electrostatic interaction for chained aliphatic odorants' accumulation tendency. Previous studies demonstrated that negatively charged functional groups were abundant in extracellular polymeric substances of sediment biofilm (Flemming et al., 2024). The lower $V_{s,\min}$ in organics usually derived from highly electronegative functional groups (e.g., carbonyl or hydroxyl groups), which are difficult to adsorb into the biofilm of the sediment due to the electrostatic repulsion (Abdeen et al., 2025). For instance, propanoic acid (Vfa2) and 2-methylpropanoic acid (Vfa3) are typical volatile fatty acids, which reported to be produced from the anaerobic metabolism of microorganism in sediment such as the isoleucine degradation by clostridium species (Zhou et al., 2024). However, the corresponding SAF values of Vfa2 and Vfa3 are much lower than those of thioethers, which might explain the decreased $V_{s,\min}$ of volatile fatty acids limiting the accumulation behaviors of these in sediments (Fig. 4). Moreover, the chained aliphatic odorant with higher E_{HOMO} can be resistant to the biodegradation in sewer sediment of anaerobic environment due to its poor electron donating capacity. Therefore, thioethers exhibited higher SAF ranging from 2.8 to 4.3, which can be attributed to their electrostatic adsorption and resistance to biodegradation.

Compared with the SAF model for chained aliphatic odorant, in SAF model for cyclic aliphatic odorant (see Eq. (4)), chemical potential (μ) has the higher coefficient value of 0.99. Similarly, μ has a high coefficient value of 0.45 in the SAF model for aromatic odorant (see Eq. (5)). μ is commonly employed to describe the energy level of organics, where higher μ means that the molecule is more likely to participate in a reaction or migrate to a more stable state (Itskowitz and Berkowitz, 1997). The higher fitted coefficient values of μ indicates that cyclic aliphatic and aromatic odorants may adsorb into sediment via chemical reactions which highlight π - π interaction due to their conjugate structure. Moreover, the SAF of aromatic odorants was also positively correlated with Windx and ShpA, as it can be seen from Eq. (4). Windx and ShpA characterize the molecular structure such as branching and symmetry degree. As shown in Supplementary Data spreadsheet, the average Windx of indoles, phenol-derivates, esters and ethers were 1.32 times higher than that of aromatic alcohols and benzene-derivatives, and thus

Table 1
Detailed QSPR models for odorants and related coefficient.

Odorant type	Descriptor	Meaning	coefficient	Variance inflation factor	P
Chained aliphatic odorants	E_{HOMO}	energy of the highest occupied orbital	0.19	2.0	<0.05
	η	orbital hardness	-0.06	2.2	<0.05
	$V_{s,\min}$	the minimal value of the molecular surface potential	0.92	2.7	<0.01
Cyclic aliphatic odorants	Topodia	topological diameter	0.20	1.9	<0.05
	E_{LUMO}	energy of the lowest unoccupied orbital	-0.02	1.7	<0.05
	V	molecular volume	0.05	1.4	<0.05
Aromatic odorants	μ	Chemical potential	0.99	7.8	<0.05
	μ	Chemical potential	0.45	1.2	<0.01
	WindX	wiener Index	0.78	1.2	<0.01
	ShpA	shape attribute	0.34	1.6	<0.05
	SVDe	sum of valence degrees	-0.02	1.7	<0.05

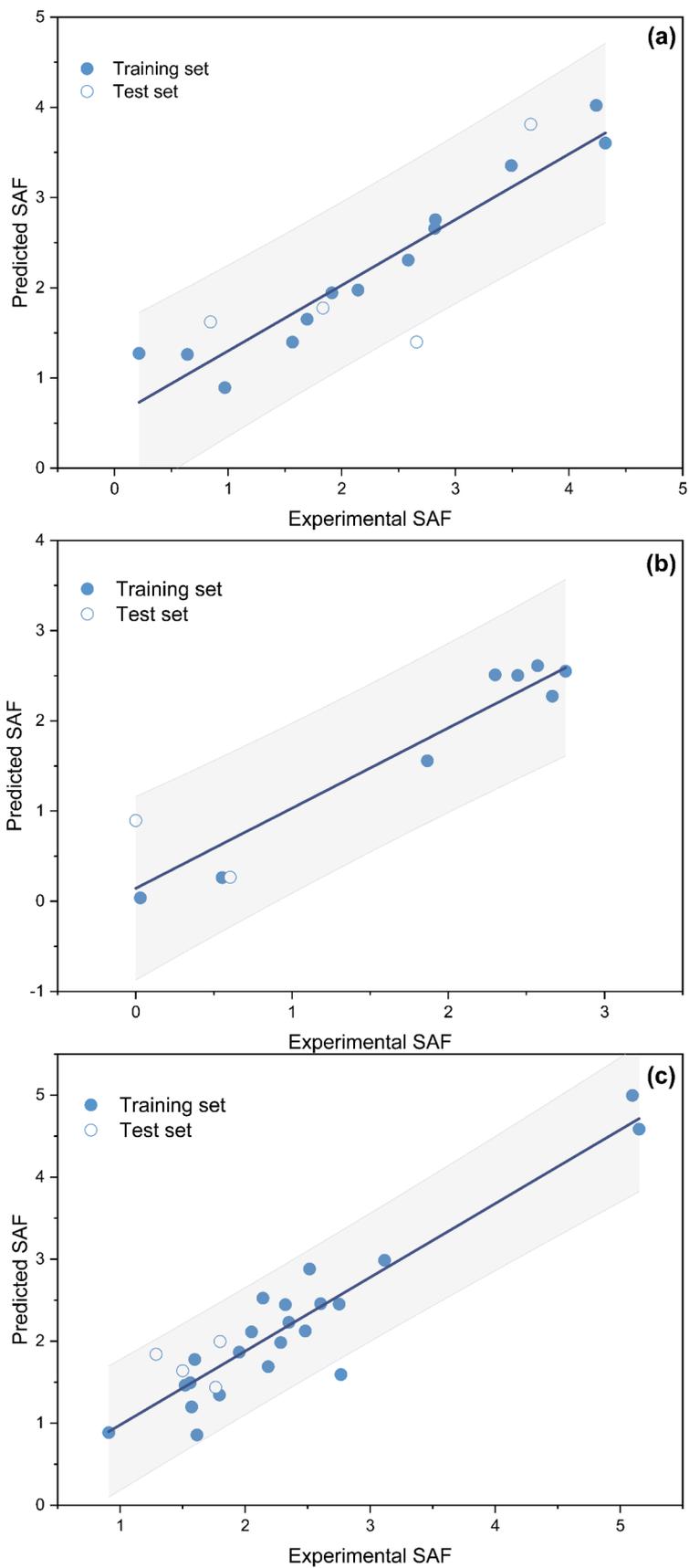


Fig. 4. Relationships between experimental and predicted SAF of (a) chained aliphatic odorant, (b) cyclic aliphatic odorant and (c) aromatic odorant in sediment.

rainfall. Chlorinated anisole and pines pose greater impacts on aquatic organisms due to their higher persistence and ecotoxicity.

This study offers a theoretical foundation and engineering guidance for pollution control strategies of storm sewer discharge during rainfall. For example, indole can serve as the precursor of chlorophenylacetoneitriles and haloacetoneitriles as toxic disinfection byproduct (Zhang et al., 2021). Therefore, the discharges of indoles from storm sewer to surface water not only cause odor nuisance, but could be also causing potential risk associated with drinking water, especially in regions where stormwater-affected waters are used as drinking water sources. Similarly, thioethers are strictly regulated odorants in drinking water. Besides, it highlights the importance of effective treatment of odorants from storm sewer discharges at the sewer end during wet weather or abatement of sewer sediment's pollutant during dry weather. For the former one, the centralized and efficient physico-chemical treatment technology is better suited for the emission dynamics across different rainfall intensities than biological technology requiring longer and more consistent hydraulic residence time. For the treatment of sewer sediment, some slow-release agents that modulate the microbial environment of sediments or degrade organic matter may be a feasible strategy, especially for the sediment-dominated odorant. Further in-depth studies on the chemical and biological assays of sewer sediments are required to better assess the risks posed by storm sewer discharges.

CRedit authorship contribution statement

Cheng Ye: Writing – original draft, Visualization, Methodology, Formal analysis, Data curation, Conceptualization. **Fangyuan Jiang:** Investigation, Funding acquisition. **Feifei Wang:** Writing – review & editing, Methodology. **Zoran Kapelan:** Writing – review & editing. **Zuxin Xu:** Funding acquisition, Conceptualization. **Michael R. Templeton:** Writing – review & editing. **Wenhai Chu:** Methodology, Investigation, Funding acquisition, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgements

This study was supported by, and received funding from National Natural Science Foundation of China (52325001, 52400114), National Key Research and Development Program of China (2021YFC3200700, 2021YFC3200702).

Supplementary materials

Supplementary material associated with this article can be found, in the online version, at [doi:10.1016/j.watres.2025.124313](https://doi.org/10.1016/j.watres.2025.124313).

Data availability

Data will be made available on request.

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