



Occurrence, migration, and ecological risk assessment of Neonicotinoid insecticides in water and sediments of Dongting Lake, China

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ABSTRACT

Neonicotinoid insecticides (NEOs) have become an integral part of the global insecticide market due to their high efficiency and low toxicity. However, their environmental persistence has raised significant ecological concerns. Dongting Lake represents a vital freshwater lake in China, and its ecosystem health directly affects regional ecological balance and people's livelihoods. This study systematically investigated the occurrence characteristics and ecological risks of NEOs in water bodies and sediments across the Dongting Lake basin. Based on surface water and sediment samples collected from 26 representative sampling sites, this study quantified nine NEOs using liquid chromatography triple quadrupole mass spectrometry. Furthermore, it assessed ecological risks posed by the NEOs using the risk quotient (RQ) method and fugacity modeling. The results revealed the presence of six NEOs in the water bodies: imidacloprid (IMI), acetamiprid (ACE), clothianidin (CLO), thiamethoxam (THIA), flonicamid (FLO), and dinotefuran (DIN). The total concentrations of these six NEOs averaged 275.11 ng/L. Five predominant NEOs (i.e., IMI, THIA, ACE, CLO, and DIN) were identified in the sediments, with a mean concentration of 0.31 ng/g. The NEO concentrations in the water bodies across the Dongting Lake basin increased in the order of the Xiangjiang, Zishui, Yuanjiang, and Lishui rivers (collectively referred to as the Four Rivers), the mainstream of Dongting Lake, the Xinqiang River, the Miluo River, and the Hudu, Ouchi, and Songzi rivers (collectively referred to as the Three Outlets). Sediments from tributaries progressively accumulate in the lake. The ecological risk assessment identified IMI and DIN as the highest-risk compounds ($RQ > 1$), with high-risk areas concentrated in the mainstream of Dongting Lake and the Ouchi, Miluo, and Hudu rivers. The fugacity model showed that IMI, ACE, and THIA are prone to diffuse from sediments to water bodies in most areas, with fugacity fractions (ff) values of greater than 0.5. In contrast, the mainstream of Dongting Lake acts as a sink of CLO and DIN (ff values: < 0.5). Sediments at the lake's outlet emerge as an important sink of NEOs. Based on the results of this study, it is advisable to strengthen the supervision of NEO applications in agricultural areas and to implement zonal control strategies. These measures will help reduce ecological risks and protect the safety of water ecosystems in the Dongting Lake region.

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1. Introduction

NEOs, neuroactive substances derived from nicotine, have gradually replaced traditional organochlorine and organophosphorus insecticides due to their insecticidal

efficacy and low toxicity to mammals, emerging as widely used insecticides worldwide (Mahai G et al., 2021; Sánchez-Bayo F et al., 2016). NEOs can interfere with neural transmission by targeting the nicotinic acetylcholine receptors (nAChRs) in insects, further leading to insect death. Additionally, their sublethal effects, including the collapse and dysfunction of pollinator populations, neurotoxicity to aquatic organisms, and the risk of biomagnification in higher vertebrates, pose threats to human health such as increased risks of adverse pregnancy outcomes, respiratory diseases, and neurological disorders (Rundlöf M et al., 2015). Statistics

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reveal that NEOs have been registered in over 120 countries and applied to more than 140 crops; by 2014, they had accounted for 25% of the global insecticide sales revenue (Chen Y et al., 2019a). China is at the forefront of NEO production and consumption, with its intensive rice cultivation driving a continuous growth in demand for NEOs (Shao X et al., 2013). Alarming, only less than 5% of the applied NEOs are absorbed by crops, while over 80% remain in the soil matrix (Hallmann C A et al., 2014). The high water solubility and low soil adsorption coefficient of NEOs facilitate their hydrological transport into aquatic systems via surface runoff and percolation (Lu C et al., 2020; Sur R and Stork A, 2003). Currently, NEOs have been frequently detected in various environmental media such as surface water (Chen Y et al., 2019b), sediments (Huang Z et al., 2020), soils (Zhang C et al., 2020), and wetlands (Main AR et al., 2014; Yu Z et al., 2021) worldwide. The geometric mean concentration of NEOs in global agricultural watersheds reaches 0.13 $\mu\text{g/L}$ (Morrissey CA et al., 2015). In the United States, at least one NEO type was detected in 53% of surface water samples. Notably, in the Great Lakes region—a major freshwater source, 74% of samples contained at least one NEO type, and 10% contained more than three, with a maximum NEO concentration reaching 230 ng/L . Studies show that most water samples from the Tagus River basin in Spain contained at least one NEO type (Casillas A et al., 2022). In the basins of major rivers in China, including the Pearl River, Huaihe River, and Poyang Lake, NEOs are commonly detected at high detection rates (Felsot A et al., 1998; Yi X et al., 2019; Zhang C et al., 2019; Zhang X et al., 2023a). Notably, NEOs in environments are governed by sediment-water interactions, with a half-life (DT_{50}) in soils reaching up to 1000 days, in contrast to 1–40 days in water bodies (Liu Z et al., 2022; Yuan B et al., 2021). Sediments act as both a sink of NEOs and a potential source of secondary pollution due to desorption. The Dongting Lake basin, a wetland and a key floodplain of the Yangtze River, is a major rice production base in China, with an annual production: exceeding 16 million tons. Agricultural production in this basin has caused large quantities of NEOs to occur in the ecological environment. Furthermore, the unique river-lake system in the basin leads to continuous NEO migration and conversion in the environment. Most studies on Dongting Lake focus predominantly on heavy metals, and recent studies have explored microplastics and antibiotics in the lake (Jiang C et al., 2018; Wang J and Yin L, 2022; Wu C et al., 2024; Zhang X et al., 2025). However, within the sedimentary system dominated by agriculture in the lake, NEO contamination is yet to be systematically investigated. Existing studies indicate that there is a lack of comprehensive data on surface water exposure to NEOs for over 90% of global agricultural regions (Stehle S et al., 2023). Although most investigations suggest that individual NEOs in aquatic environments carry low ecological risks, exposure to mixed NEOs poses chronic risks to aquatic invertebrates. Prolonged exposure may potentially threaten the health of humans and

ecosystems (Liu Z et al., 2021; Zhang X et al., 2023b).

This study systematically investigated NEOs in the water-sediment system in the Dongting Lake basin. It determined the spatial distribution patterns of NEOs in the Three Outlets and the Four Rivers and assessed their ecological risks. The sediment-water partitioning mechanisms modulated by alluvial sediments were analyzed using a level III multimedia environmental model. Furthermore, this study summarized the distribution and migration characteristics of NEOs in the water environments of distinct zones in the Dongting Lake region and proposed recommendations for zone-specific management and control. The findings of this study will advance the understanding of insecticide behavior in complex floodplain ecosystems and provide key insights into the balance between agricultural productivity and ecological security in sedimentary basins.

2. Materials and methods

2.1. Overview of the study area and sample collection

The Dongting Lake region, located in the middle reaches of the Yangtze River basin, covers a total area of approximately 37000 km^2 . As the second largest freshwater lake in China, Dongting Lake plays a crucial role in regulating and storing water within the Yangtze River basin. This lake collects water from the Four Rivers in the south and receives floodwater from the Yangtze River through the Three Outlets in the north. Additionally, Dongting Lake is connected to the Miluo and Xinqiang rivers in the east, ultimately flowing into the Yangtze River at Chenglingji in Yueyang City. The unique geographical location of the Dongting Lake contributes to the formation of complex, delicate river-lake relationships. To thoroughly investigate the relationship between the geographical distribution of Dongting Lake and agricultural production, this study conducted field surveys of 26 representative sites that were meticulously selected for sampling. To collect comprehensive data on river water quality and sediments, sampling sites were arranged in the four major rivers, including S1-S3 in the Xiangjiang River, S4-S7 in the Zishui River, S8-S11 in the Yuanjiang River, and S12-S15 in the Lishui River. Sampling sites S17-S20 were deployed in the Songzi, Hudu, Ouchi, Miluo, and Xinqiang rivers, respectively, with one sampling site arranged in one river. To explore the characteristics of water quality and sediments in Dongting Lake, five sampling sites (i.e., S21-S25) were set within the lake. Additionally, sampling site S26 was arranged at the location where Dongting Lake flows into the Yangtze River to obtain comprehensive data on changes in the water quality in the lake region.

During water sampling, open areas with steady flow in rivers were selected to ensure that representative water samples were obtained. Brown glass sample bottles were used for sampling. Two bottles of water samples, each with a capacity of 1 L, were collected at a position about 30 cm below the water surface. Then, screw caps lined with polytetrafluoroethylene membranes were quickly screwed

onto the bottles to prevent the collected samples from being contaminated by external sources. To minimize the impacts of evaporation and gas exchange, the bottles were filled with water samples, with no space left above the liquid. Sediment samples were collected near the water samples using grab samplers and were then transferred to 250 ml brown glass wide-mouth bottles. To ensure the purity of the sediment samples, the sampler was gently tilted to allow water in the upper part to drain out slowly during the sample transfer. After being filled with sediments, the bottles were immediately sealed to prevent contamination. In the case where sediments had high water content, at least 100 g of solid sediments were collected to ensure the accuracy of the analysis. All the samples were sent to the laboratory for preprocessing within 24 h of collection and were analyzed within five days to ensure the data accuracy and reliability.

2.2. Sample processing and chemical analysis

Treatment and analysis procedure for water samples: After being shaken evenly, water samples precisely measuring 4.5 mL were removed and were then mixed thoroughly with 0.5 mL of methanol. The resulting mixture was filtered using a filter membrane with a 0.22 μm pore size. To minimize possible contamination and interference, the first 2 mL of filtrate was discarded. 10 mL of the filtered samples were transferred to a brown vial, to which 10 μL of internal standard solution was added. Then, the samples were mixed thoroughly for analysis.

Treatment and analysis procedure for sediment samples: sediment samples weighing approximately 20 g were placed in a 150 mL conical flask. After 5 mL of distilled water and 50 mL of acetonitrile solution were added, the samples were shaken at 25°C for 1 h using a temperature-controlled shaker. Then, the samples were filtered using a vacuum filtration apparatus, and the filtrate collected was transferred to a 100 mL graduated cylinder with a stopper, to which 5 g of sodium chloride was added. Afterward, the filtrate was manually shaken for 1 min and was then kept undisturbed for 5–10 min. The supernatant measuring 25 mL was placed in a 100 mL round-bottom flask and was then concentrated to dryness at 40°C in a rotary evaporator. Subsequently, the concentrated samples were reconstituted using 5 mL of acetonitrile for purification. All the samples reconstituted using acetonitrile were transferred onto an HLB solid-phase extraction column, which was activated and equilibrated using 2 mL of dichloromethane and 2 mL of water in advance. After the samples were eluted three times using 5 mL of dichloromethane, they were concentrated to dryness at 40°C. The concentrated samples were reconstituted using 1 mL of acetonitrile and were then filtered using a 0.22 μm filter membrane. Then, a certain amount of internal standard solution was added to the samples and mixed thoroughly. Finally, the prepared samples were placed in the detection instrument for quantitative analysis using the internal standard method.

Chromatography and mass spectrometry instrumental techniques: Two mobile phases were used. Among them, Phase A was a formic acid–formic ammonium buffer solution, while Phase B was acetonitrile. The gradient elution protocol is detailed in Table S1. The flow rate was set at 0.35 mL/min, the column temperature was maintained at 40°C, and the volume of the injected samples was 20 μL . The mass spectrometer operated in positive ion mode, with an ion source voltage of 4500 V and an ion source temperature of 600°C. The nebulizer gas pressure (GS1) and the heated auxiliary gas pressure (GS2) were both set at 60 psi, while the curtain gas pressure was at 30 psi. The multiple reaction monitoring (MRM) detection mode was used.

2.3. Quality control

A liquid chromatography triple quadrupole mass spectrometer with higher precision was selected to detect the nine NEOs. All items were validated using the laboratory methods specified in the *Technical guideline for the development of environmental monitoring analytical method standards* (HJ168-2020). The detection limits, accuracy, and precision of the methods all met the relevant regulations and requirements. Prior to sample analysis, no target NEOs were detected in the blank samples, and alternative internal standards THIA-d3 and IMI-d4 were added to monitor the sample preparation process. The method detection limits (MDLs) for the target analytes in the samples are described in Supplementary Table S2. In this study, the recovery rates of the nine target compounds ranged from 80% to 120% in water and from 70% to 130% in sediments.

2.4. Ecological risk assessment

RQ is recognized as the most widely utilized method for characterizing the ecological risks posed by pollutants. Based on the *Technical Guidance Document* (TGD) for risk assessment of chemical substances issued by the European Union, the RQ value can be determined by comparing the measured environmental concentration (MEC) of a pollutant with the predicted no-effect concentration (PNEC), as shown in Equation (1):

$$\text{RQ} = \text{MEC}/\text{PNEC} \quad (1)$$

where RQ is the risk quotient, dimensionless; MEC is the measured environmental concentration, $\text{ng}\cdot\text{L}^{-1}$, and PNEC is the predicted no effect concentration, $\text{ng}\cdot\text{L}^{-1}$, as referenced in existing studies (Table S3). RQ values of greater than 1, 0.1–1, and less than 0.1 indicate the presence of risks, the presence of potential risks, and no risk, respectively.

2.5. Migration trends in sediments and water

The level III multimedia environmental fate model is commonly employed to simulate pollutant migration across varying environmental compartments. This model considers multiple processes such as volatilization, deposition,

biodegradation, adsorption, and desorption. The calculation process is detailed in the Supplementary Material (Text S1). In this study, the fugacity fraction (ff) was used as an indicator. A fugacity fraction value of greater than 0.5 denotes that NEOs are prone to migrate from sediments to the water. In this case, sediments act as a secondary source for NEO release. Conversely, when ff is less than 0.5, sediments serve as a sink, and NEOs tend to diffuse from water into sediments.

3. Results and discussion

3.1. Detection of NEOs in water and sediments of Dongting Lake

The spatial distributions of nine target NEOs in water and sediments of the Dongting Lake region (Fig. 1) reveal the presence of six NEOs in water: IMI, ACE, CLO, THIA, FLO, and DIN. In contrast, NIT, THI, and IMID were not detected in water. The six detected NEOs exhibited concentrations in water ranging from 101.4 ng/L to 1094.7 ng/L across 26 sampling sites, with an average of 271.5 ng/L. At these sites, ACE, CLO, THIA, and DIN were detected in all samples, suggesting their frequent application in the Dongting Lake region. IMI showed a detection rate of 46%, while FLO was detected only at a few sites. THIA exhibited the highest average concentration of 657.2 ng/L, followed by IMI (206.0 ng/L). Both insecticides had average concentrations exceeding 100 ng/L, establishing them as the cause of concern when compared to the recommended risk thresholds of IMI and THIA in surface water of China (acute and chronic risk thresholds of IMI: 8 ng/L and 30 ng/L, respectively; acute and chronic risk thresholds of THIA: 150 ng/L and 420 ng/L, respectively). Five NEOs were detected in sediments. Among these, THIA exhibited a detection rate of 100%, followed by ACE (96%), IMI (77%), CLO (65%), and DIN (58%). These NEOs exhibited concentrations in sediments varying from 0.02 ng/g to 1.09 ng/g across 26 sampling sites ($n = 26$), with an average of 0.31 ng/g. THIA and IMI exhibited the highest

average concentrations in sediments, mirroring their distributions in water.

The compositions of NEOs in water and sediments at various sampling sites in the Dongting Lake region indicate that water and sediments exhibit roughly the same primary NEO constituents, which are dominated by IMI, THIA, and ACE. This occurs because formulations with IMI, THIA, and ACE as active ingredients have been registered more extensively in China compared to the remaining six NEOs. Among the nine NEOs, active ingredients IMI and THIA represent the most widely used insecticides. IMI, a first-generation NEO and one of the most widely used insecticides globally, shows high detection rates and concentrations in water environments across varying countries and regions (Liu Z et al., 2021). Although THIA is less immediately effective than IMI, it offers the advantages of a broad insecticidal spectrum, high systemic activity, and long-lasting effects. Therefore, compared to other NEOs, these two components have higher detection rates and residual concentration levels in an aquatic environment. DIN is more prevalent in water than in sediments, and the possible reason is that DIN is a third-generation NEO and is applied less frequently than the first- and second-generation insecticides. The migration and persistence of DIN in an aquatic environment are yet to be fully understood.

3.2. Characterization of NEOs in water and sediments of Dongting Lake

The compositional characteristics of NEOs in rivers and sediments (Fig. 2) at various locations within the Dongting Lake region reveal that NEOs were detected in the water and sediment samples from all rivers, exhibiting varying degrees of contamination. The NEO concentrations in the water bodies of the lake increased in the order of the Four Rivers, the mainstream of Dongting Lake, the Xinqiang River, the Miluo River, and the Three Outlets. The Four Rivers exhibited relatively low NEO concentrations in water, with the total NEO concentrations varying slightly between

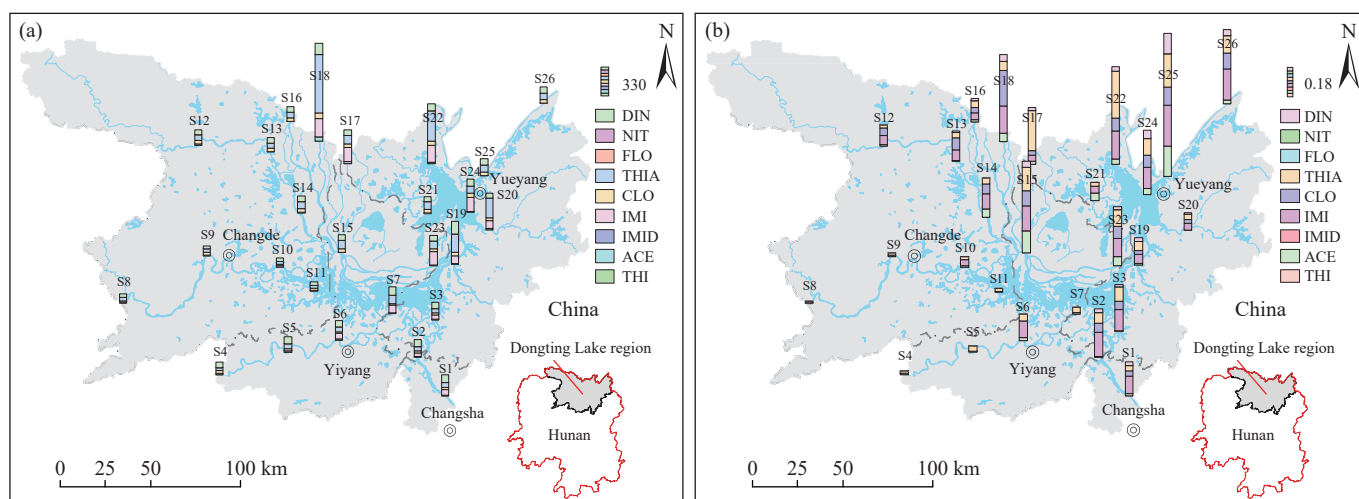


Fig. 1. Spatial distributions of NEOs in water (a) and sediments (b) of Dongting Lake.

different rivers and showing a gently increasing trend from the upper to lower reaches. The NEO concentrations in water in the Xinqiang River, the MiLuo River, and the Three Outlets were higher than those in the mainstream of Dongting Lake, suggesting that the primary rivers produce higher dilution effects than secondary rivers, with pollutants ultimately converging into the lake. The five sediment samples from Dongting Lake exhibited an average NEO concentration of 0.58 ng/g, which is generally higher than that in sediments in other rivers. This finding indicates a widespread presence of NEOs in the lake body. The Four rivers exhibited gradually increasing NEO concentrations in sediments from the upper to lower reaches, signifying gradual NEO accumulation in river and lake sediments. The elevated NEO concentrations in sediments in the lake suggest that NEOs are enriched in both the water column and sediments. Therefore, the NEO concentrations in water bodies reflect the level of environmental contamination around rivers, while those in sediments can indicate the temporal enrichment characteristics of NEOs more effectively. The consistency between the distribution patterns in water and sediment samples further underscores the scale of NEO contamination. Among the rivers surveyed and their sediments, the Yuanjiang River showed the lowest level of NEO contamination, while the highest NEO concentration was observed in the Ouchi River. The Xiang and Yangtze rivers are significant contributors to Dongting Lake. Notably, in the Xiangjiang River, the NEO concentration in water was significantly lower than that in sediments, implying that the NEO enrichment in sediments can reflect the level of regional NEO contamination more accurately. In contrast, the MiLuo River exhibited more severe water pollution, with the temporal NEO accumulation significantly lower than that in other inflowing rivers.

The distributions of individual NEOs in the rivers of Dongting Lake (Fig. 3) reveal that THIA was the predominant NEO in water, accounting for 40% of the total NEOs (\sum NEO) in water on average, followed by DIN, which represented 25.5% of total NEOs. In the sediments, IMI and THIA were identified as the primary contributors to NEOs, with average concentrations of 0.13 ng/g and 0.09 ng/g, respectively and accounting for 33.3% and 29.0% of the total NEOs in sediments. These two insecticides were also abundant in water, indicating a consistency in residual NEO distributions between water and sediments. The peak NEO concentration in water was observed at site S18. This might be attributed to factors such as hydrological conditions, flow velocity, or the distribution of surrounding pollution sources. The five sampling sites of water in Dongting Lake exhibited an average concentration of total NEOs in water of 352.0 ng/L, with the NEO concentrations varying slightly across various sites. This suggests that the overall level of NEO contamination in water remained relatively stable in the lake and that the degrees of contamination appeared similar across the sampling sites. Site S25 (186.9 ng/L), located at the estuary where Dongting Lake flows into the Yangtze River, showed a similar concentration in water to site S26 (182.3

ng/L) situated in the Yangtze River, both lower than the average concentration of total NEOs in Dongting Lake. This indicates that water exchange between Dongting Lake and the Yangtze River has influenced the NEO distribution, producing a dilution effect at site S25 near the estuary and its adjacent site S26. The peak concentration in sediments was observed at site S25, while sites S22 and S15 also exhibited high NEO concentrations. This could be attributed to the fact that site S22 was located in the northeastern part of Dongting Lake, where the relatively stable hydrological environment facilitated NEO accumulation in sediments. Meanwhile, site S15 was at the confluence of the Lishui River and the Three Outlets, where pollutants accumulated significantly. This further underscores the important influence of geographical environments and flow conditions in varying areas on the NEO distribution in sediments. Additionally, the convergence of different water systems or unique hydrological conditions can lead to considerable variations in NEO accumulation in sediments.

3.3. Risk assessment

The ecological risks posed by the five major NEOs detected in Dongting Lake water were assessed using the RQ method (Table S4). The assessment results indicate that all the five NEOs exhibited RQ values of greater than 0.1, indicating the presence of potential or high risks. IMI and DIN posed the highest risk in the water. Among these, DIN showed RQ values of greater than 1 in all areas, confirming its risky nature. Although the RQ values of IMI varied widely, they exhibited a maximum of up to 20.6. Since the maximum is far greater than 1, IMI posed high risks in the study area.

The heatmap plotted based on the RQ values of NEOs of varying sampling points (Fig. 4) reveals that the study area can be categorized into three types: high-risk areas requiring urgent actions ($RQ > 15$), medium-risk areas requiring constant

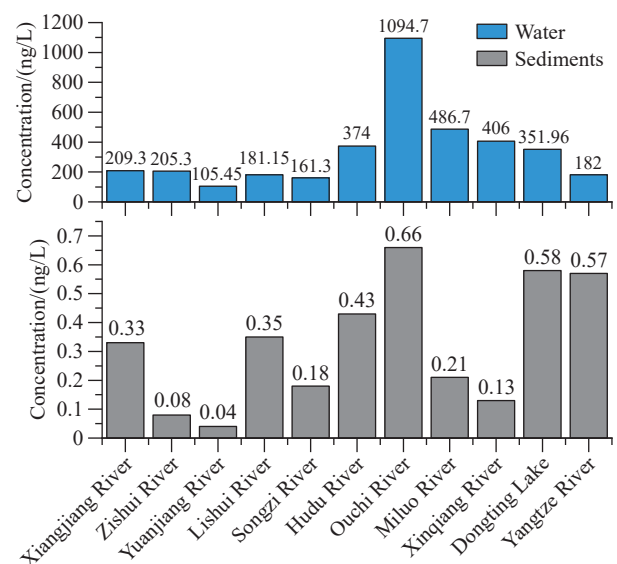


Fig. 2. Levels of NEO concentration in water and sediments of Dongting Lake.

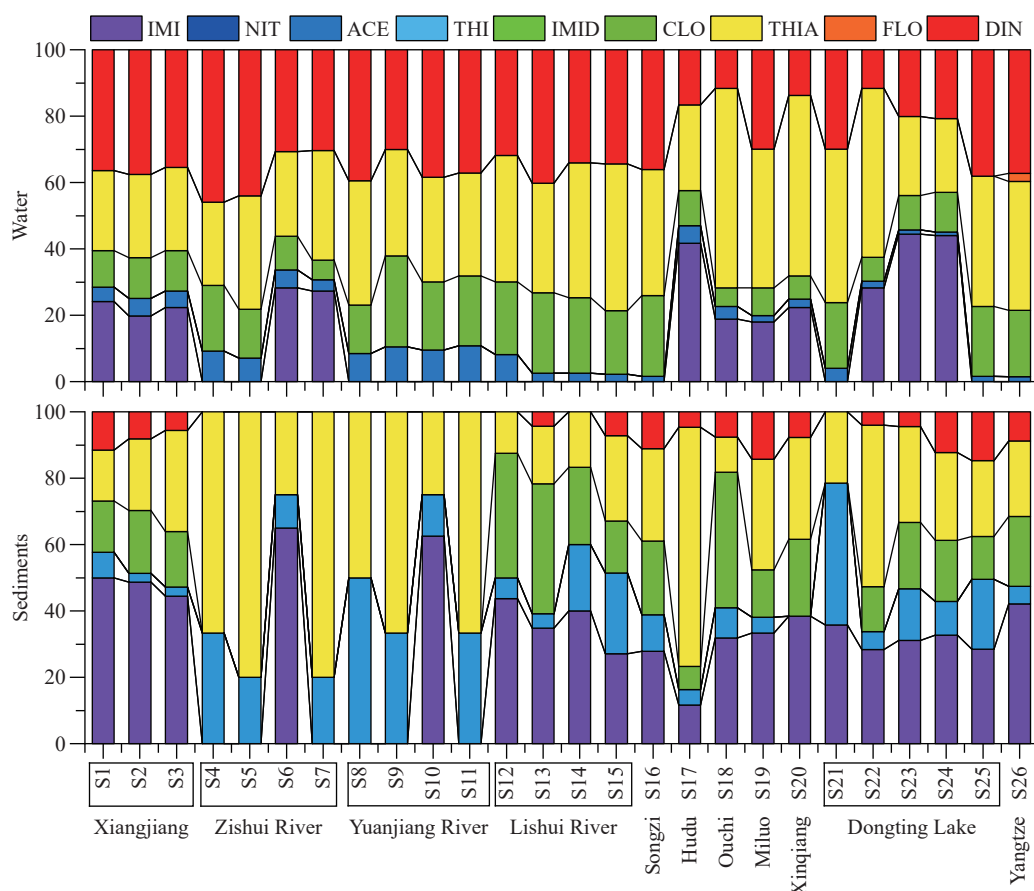


Fig. 3. Concentrations of individual NEOs in water and sediments of Dongting Lake.

monitoring ($5 \leq RQ \leq 15$), and low-risk areas ($RQ < 5$). The high-risk areas include the Ouchi River, the mainstream of Dongting Lake, the Miluo River, and the Hudu River. In the Ouchi River—an inflow river, the high risks might be associated with the extensive application of IMI in the agricultural area along the upper reaches. In this river, IMI, THIA, and DIN contribute significantly to the RQ values, posing serious threats to fish and benthic organisms. In the mainstream of Dongting Lake, the pollution reflects the cumulative effect of inputs into the river basin. IMI and DIN contribute the most significantly, posing a threat to the wetland ecosystem. In the Miluo River and the Hudu River (a tributary of the Yangtze River), the high IMI and DIN concentrations might affect the ecology in the lower reaches of the Yangtze River through the food chain. The medium-risk areas involve the Xinjiang, Zishui, Xiangjiang, Lishui, and Yangtze rivers, where CLO and DIN pose high ecological risks. The Lishui River is located in the middle to upper reaches with agricultural activities, from which the continuous CLO input might produce sublethal effects on crustaceans. The sampling point was arranged at the confluence of the Yangtze River and Dongting Lake, where pollutant diffusion might affect the mainstream of the Yangtze River. Studies have indicated the presence of high risks in the Yangtze River. The low-risk areas include the Yuanjiang and Songzi rivers. The Yuanjiang River exhibited local hotspots of insecticide application, rendering it necessary to take

precautions against the risks of increasing NEO concentrations in the rainy season. The relatively low NEO concentrations in these river basins reflect the effectiveness of current management. The high risks in Dongting Lake necessitate investigating the pollution sources in time, restricting the application of highly toxic insecticides, and normalizing insecticide application rules. Generally, the ecological risks posed by NEOs in the water bodies of Dongting Lake feature multi-point outbreaks and local extremely high concentrations. Therefore, it is advisable to adopt a risk response strategy of zonal control and pollutant treatment prioritized.

3.4. Migration patterns of NEOs in water and sediments of Dongting Lake

The migration patterns of NEOs in water and sediments affect the distributions of these compounds. This study quantified these patterns using a fugacity model and analyzed the fugacity distributions of five pollutants (i.e., IMI, ACE, CLO, THIA, and DIN) in 11 sub-basins of the Dongting Lake basin (Table S6). The analytical results indicate that the migration trends of the five NEOs vary across various sub-basins (Fig. 5). At most sampling points across the entire basin, IMI, ACE, and THIA exhibited *ff* values of greater than 0.5, indicating their high enrichment in sediments and the widespread diffusion of IMI and ACE. In 75% of the samples, CLO and DIN exhibited *ff* values of less than 0.5. The *ff*

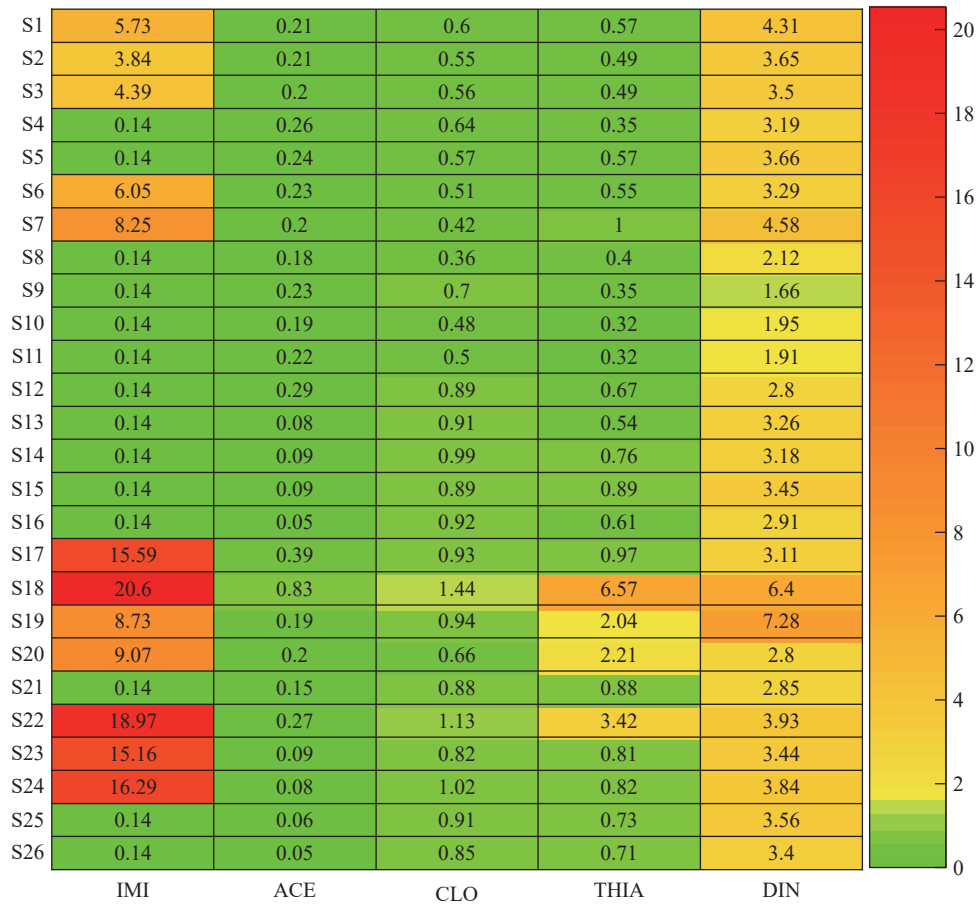


Fig. 4. Heatmap of RQ values of NEOs in water of Dongting Lake.

distributions of NEOs at the sampling points reveal that the mainstream of Dongting Lake acts as a sink of pollutants such as DIN and CLO, which exhibited significantly higher ff values in the lake than in its tributaries. The discussion of various areas reveals higher ff values of IMI (0.81–0.90) and THIA (0.63–0.84) in the Xiangjiang River. This might be related to the frequent applications of IMI and THIA in rice fields along the river banks. In the Zishui River, IMI generally showed very high ff values, except that (0.03) at site S7. This finding suggests strong degradation or dilution effects in local areas. In this river, CLO and DIN exhibited the lowest ff values, varying from 0.13 to 0.18 and from 0.11 to 0.18, respectively. This reflects the weak mobility of the two compounds in water. In the Yuanjiang River basin, the stable, high ff values of IMI and ACE indicate the predominance of sediment adsorption. Furthermore, a negative correlation was observed between the ff values of CLO and THIA, suggesting the potential presence of competitive migration between them. In the Lishui River basin, ACE (ff values: 0.9167 at S14 and 0.9733 at S15) and IMI (ff values: > 0.99) were nearly saturated, indicating high ACE and IMI enrichment in the sediments. In Dongting Lake and its outlet (S21–S26), all the five pollutants exhibited ff values of greater than 0.72. This could be attributed to the fact that the high sediment content facilitates NEO adsorption, reflecting that sediments serve as a sink of NEOs in sediments at the lake's outlet. Compared to other areas, Dongting Lake shows significantly lower ff

values of CLO. This might be associated with the accelerated migration of the compound due to water flow.

In combination with the sampling points and the fugacity fraction values of NEOs, this study conducted a cluster analysis (Fig. 6). As a result, four types of typical areas were determined: agriculture-dominated areas, sediment-enriched areas, mixed pollution areas, and low-risk areas. For these areas, this study proposed corresponding measures. The agriculture-dominated areas are characterized by high ff values of IMI and THIA and a low fugacity fraction value of CLO (0.18). In these areas, 80% of the samples were collected from the Xiangjiang and Yuanjiang rivers, and the river basins are typical agricultural areas with intensive rice cultivation. For these areas, it is advisable to restrict the applications of IMI and THIA during the planting season. The sediment-enriched areas show high ff values of ACE (0.93) and CLO (0.67). In these areas, 60% of samples were collected from the mainstream of Dongting Lake and the inlet of the Yangtze River. It can be inferred from these samples that the lake's outlet is adjacent to zones with high sediment retention. Therefore, it is recommended to conduct regular sediment treatment for these areas. The mixed pollution areas exhibit moderate concentrations of all the NEO compounds, with ACE and DIN showing ff values of 0.58 and 0.38, respectively. In these areas, 70% of samples were collected from the Lishui River and its secondary tributaries, and the land use near the river basins is dominated by mixed urban

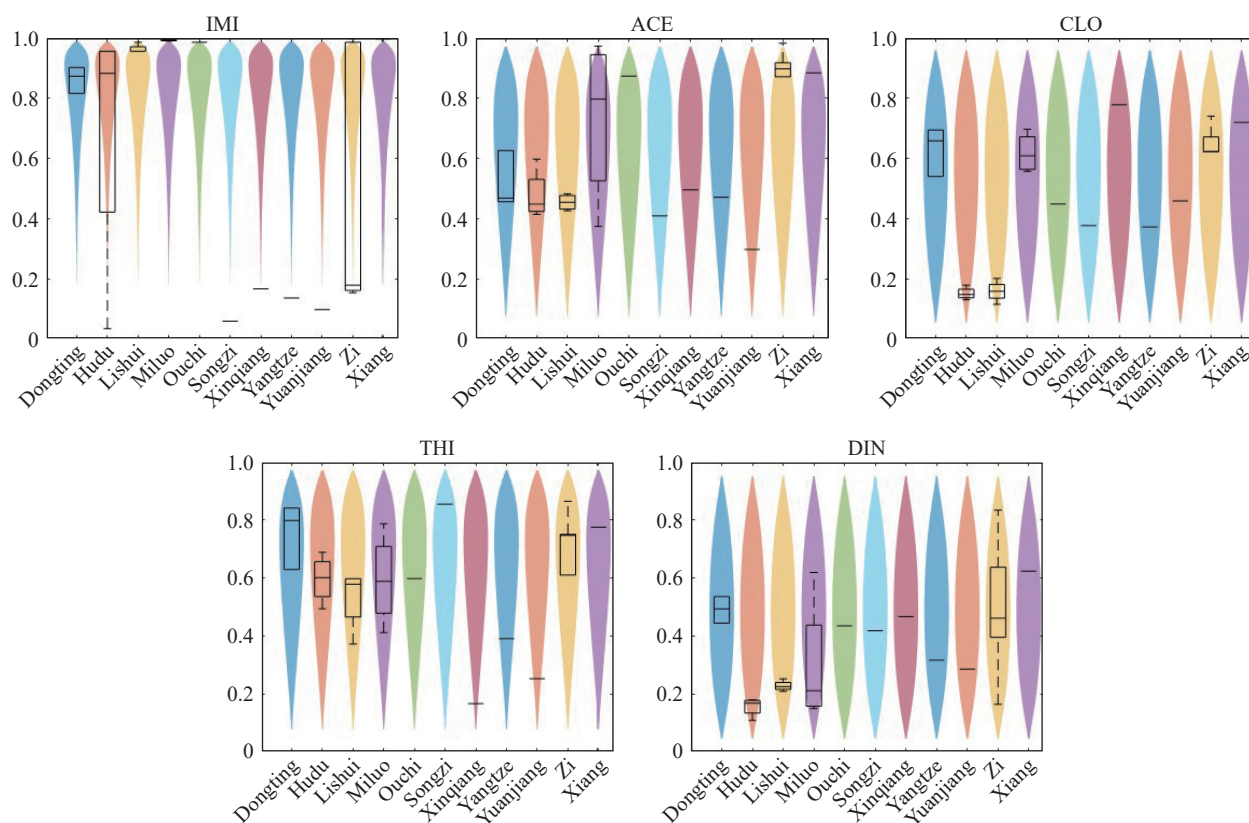


Fig. 5. Violins showing the fugacity fraction distributions of NEOs in the Dongting Lake basin.

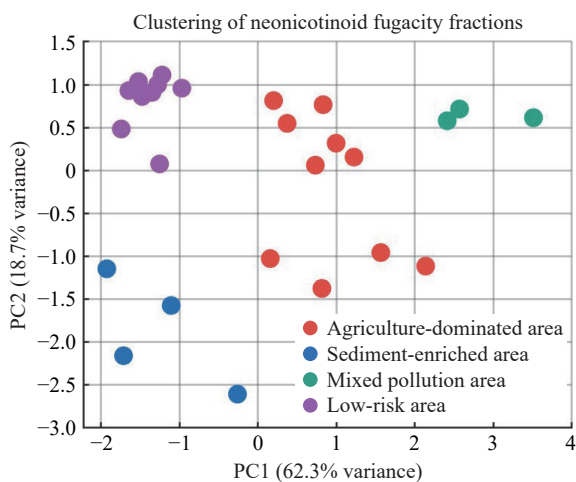


Fig. 6. Clustering of the fugacity fraction values of NEOs in the Dongting Lake basin.

and agricultural activities. For these areas, it is recommended to identify and trace pollution sources and implement vegetation coverage along the tributaries. The low-risk areas feature low fugacity fraction values of all the NEO compounds. In these areas, 90% of the samples were collected from the Hudu and Xinjiang rivers. These areas are dominated by mountainous rivers, with a sparse population. For these areas, it is necessary to conduct water quality monitoring every six months and develop ecotourism to restrict new agricultural projects. This study analyzed the characteristics and migration trends of pollutants across various areas based

on the clustering of ff values, providing targeted measures for regional management.

4. Conclusions

(i) IMI, THIA, and ACE are identified as the predominant NEOs in the Dongting Lake region. The spatial distributions of the three compounds are closely related to the intensity of regional agricultural activities and the functional characteristics of insecticides. The NEO concentrations in the water are significantly affected by the dilution effect of the mainstream, while sediment pollution shows an accumulative trend. Furthermore, the lake body exhibits higher pollution levels than the tributaries.

(ii) NEOs pose a serious threat to aquatic invertebrates in the Dongting Lake region. The high-risk areas are concentrated in the Ouchi River, the Miluo River, and the mainstream of Dongting Lake, with the RQ values (up to 20.6) of IMI and DIN far exceeding their thresholds. Therefore, there is an urgent need to prioritize the management and control of these areas.

(iii) In most areas of the Dongting Lake region, IMI, ACE, and THIA tend to continuously diffuse through sediment-water interactions (fugacity fraction values: >0.5), while CLO and DIN are more prone to be deposited in the mainstream (fugacity fraction values: <0.5). The lake’s outlet exhibits high sediment content, further enhancing the role of sediments as a sink of NEOs.

(iv) Based on the findings, it is recommended to implement zonal control strategies tailored to regional

characteristics such as agriculture predominance and sediment enrichment. These strategies include restricting the use of highly toxic NEOs, strengthening sediment dredging at the lake's outlet, and constructing ecological restoration projects. These measures will help reduce the long-term risks to the aquatic ecosystem posed by NEOs and provide a scientific basis for the control of insecticide pollution in the agricultural areas of Dongting Lake.

CRedit authorship contribution statement

Xiong Mao, Zhi-Tao Huo, and Jun Guo conceived of the presented idea. Xiong Mao and Yi Huang performed data analysis and summarization. Cong Li and Feng-cun Huang conducted field surveys and sample collection. All authors discussed the results and contributed to the final manuscript.

Declaration of competing interest

The authors declare no conflicts of interest.

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Supplementary dataset

Supplementary data (Tables S1–S6; Text S1) to this article can be found online at doi: [10.31035/cg20250037](https://doi.org/10.31035/cg20250037).

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