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Diffusive Behavior of Pollutants in Soil Environmental Water at the Microscopic Scale

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Abstract:
With the popularization of organic food and the rise of organic agriculture, the attention to soil safety issues is increasing. This study aims to thoroughly investigate the diffusion behavior of waterborne pollutants and organic contaminants in the soil environment at a microscopic scale and their long-term effects on the soil ecosystem. By establishing multiple soil-water-pollutant variable models and employing molecular dynamics simulation methods, the interaction among soil, water, and organic pollutants was systematically studied. The research findings indicate that, under low concentration conditions, anthracene molecules exhibit a wider diffusion range and stronger diffusion capability compared to naphthalene molecules; whereas under high concentration conditions, the diffusion capability of naphthalene molecules becomes more pronounced. Furthermore, in mixed pollutant systems, a competitive adsorption phenomenon occurs between naphthalene and anthracene, leading to changes in the adsorption selectivity of pollutants on the soil surface, which significantly influences the pollution spreading pathways in soil. Through in-depth research at the microscale, we have not only provided a new perspective for understanding the mechanism of waterborne pollutant diffusion in the soil environment but also laid a scientific foundation for the formulation of future environmental management policies.

Keywords: soil ecosystem; molecular dynamics simulation methods; diffusion; competitive adsorption

1. Introduction

In today's society, organly affects the growth of crops and human health[1,2]. The spread of water pollutants and organic pollutants in soil has become an urgent environmental issue that needs to be addressed globally[3-6]. To deal with that, solving organic pollutants in soil environment water and the diffusion behavior of pollutants has become a common topic of concern for environmental protectionists.

For exploring the long-term influence of the diffusion behavior of pollutants and organic pollutants in soil environmental water on the soil environment [7,8], investigating the physicochemical properties of pollutants can help us to reveal the propagation mechanism of pollutants in the soil, can better help reveal their solubility in soil, adsorption characteristics and interaction with soil particles. Beyond that, the structure of the soil and the properties of water molecules are also important factors that affect the diffusion of pollutants. It is the structure, texture of the soil, and the characteristics of water molecules moving collectively that determine the transport pathways of pollutants in the soil [9,10]. Through the research of these factors, in this paper, we can predict and control the diffusion process of pollutants more accurately. In organic agriculture, irrigation is also an indispensable part of irrigation is also an indispensable part of plant growth [11]. Therefore, investigating the interaction between soil, water, and organic pollutants is also significant for ensuring the sustainability and environmental friendliness of organic agriculture. By in-depth analysis of the microscopic relationships between these elements, we can understand the complex interaction between them at the molecular level, providing a scientific basis for the healthy development of organic agriculture.

In this study, a molecular dynamics simulation method was adopted [12,13] to explore the interaction among soil, water, and organic pollutants at the microscopic perspective. Compared with the traditional macroscopic Newtonian mechanics perspective, the microscopic perspective can provide a deeper and more comprehensive understanding and help us discover new solutions to deal with soil pollution problems. This investigation is expected to provide a new perspective for understanding the basic mechanism of environmental change, provide a scientific basis for formulating effective environmental management policies, help protect the integrity of soil ecosystems, promote the sustainable development of agriculture [14], and at the same time contribute to global environmental protection and public health security.

2. Methods

2.1 Models

Five soil-water-pollutant variable models were constructed, which contain two anthracene molecules, two naphthalene molecules, ten anthracene molecules, ten naphthalene molecules, and a mixed system containing two anthracene molecules and two naphthalene molecules. Each system includes a tip3p water model, with each model containing 500 water molecules. The soil model uses a silicon dioxide unit cell ($\alpha = \beta = \gamma = 90°$) to construct a quartz (1 0 0) surface, generating a 3 × 3 supercell (4.280 nm × 4.910 nm × 2.140 nm), and three-dimensional periodic boundary conditions are applied in the XYZ direction to form a complete three-dimensional model. After completing the construction of the soil silicon dioxide model, the tip3p water model is established, and five groups of variable models are set up to study in depth the impact of different substances and dosages on the diffusion and influence range in the tip3p water model.

To better describe the interaction between the soil and water surfaces, in the silicon dioxide surface model, a series of surface treatment steps such as the addition of hydrogen atoms to the surface are carried out, resulting in some silicon and oxygen atoms being in an unsaturated state. The specific method of addition can refer to the detailed introduction by Kleestorfer [15] and others, as well as Zhuo [16] and others. This model can be used to deeply study the diffusion of pollutants in water under different substances and dosages, as well as the interaction between pollutants and silicon dioxide. It explores the diffusion mechanism of pollutant molecules and water molecules under different pollutant conditions, thereby revealing the microscopic processes between water and soil under complex environmental conditions.

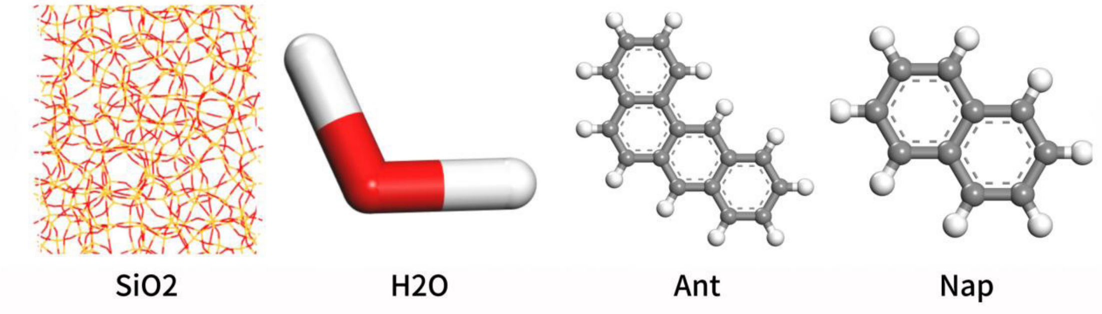

Figure 1: Schematic Diagram of Molecular Model Structure

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2.2 Method

In the simulation of the five systems, the soil (silicon dioxide) and pollutants all use the PCFF force field to calculate the non-bond energy of atoms, and water uses the tip3p model. This is because a large number of experiments have shown that this force field can accurately predict the structure, conformation, vibration, and thermophysical properties of various molecules in isolated systems or condensed systems over a wide range of temperatures and pressures. It is widely used for predicting the adsorption performance of both organic and inorganic substances. The NVT ensemble is used for molecular dynamics simulation of the above-simulated adsorption systems. A Nose thermostat is used to control the temperature at 298 K. First, a 10 ps equilibrium simulation is performed to stabilize the energy and temperature of the simulated system; then, a 200 ps dynamics simulation is carried out, saving the atomic motion trajectory file and outputting results every 1 ps.

3. Result and discussion

3.1 The impact of different pollutants on soil water at low concentrations

In Figure 2, snapshots of the model structures of different pollutants at low concentrations are shown. It can be observed that anthracene molecules exhibit a larger diffusion range compared to naphthalene molecules, a phenomenon mainly attributed to the lower molecular weight of anthracene molecules. According to diffusion theory, compounds with lower molecular weights typically have higher diffusion rates in aqueous media, hence anthracene molecules demonstrate stronger diffusion capabilities.

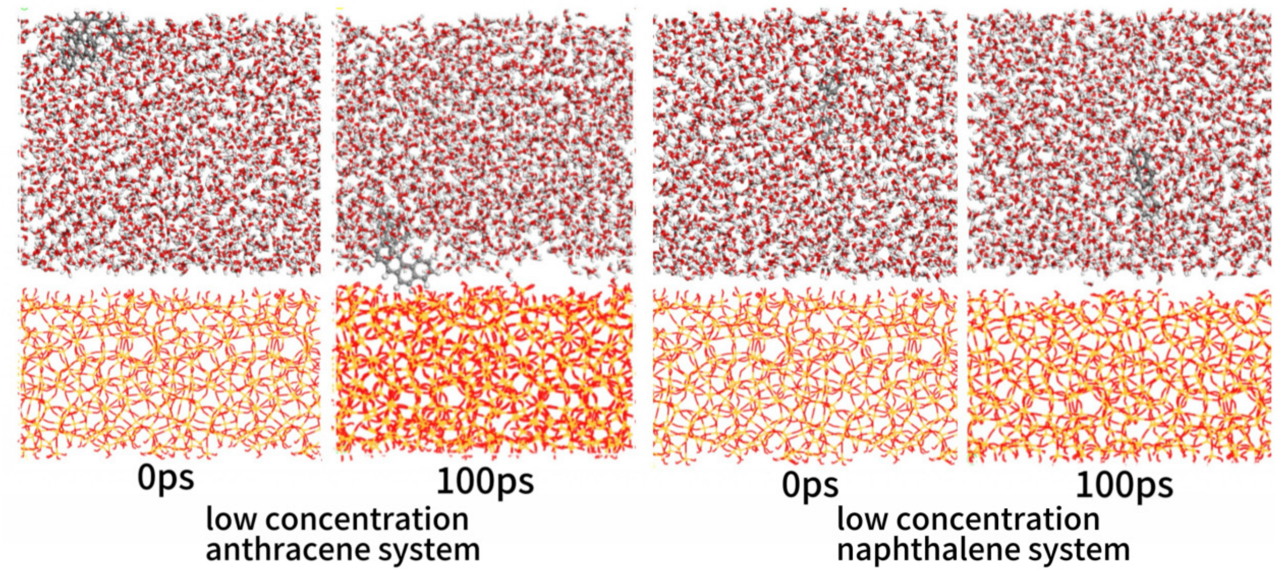

Figure 2: Snapshots of Model Structures of Different Pollutants at Low Concentration

By monitoring the energy changes in the system, as shown in Figure 3 which illustrates the energy change graph of different pollutants at low concentrations, we can gain a deeper understanding of the interaction between pollutants and the SiO_2 surface. Experimental data indicates that in the low-concentration naphthalene system, there is a significant drop in potential energy at the 50 picoseconds (ps) mark, suggesting that naphthalene molecules adsorbed onto the SiO_2 surface at this moment, leading to a decrease in potential energy. This suggests that under low-concentration conditions, naphthalene molecules are more likely to interact with the soil surface. In contrast, in the low-concentration anthracene system, the reduction in potential energy is slower, and before the 50 ps mark, its total potential energy is lower than that of the low-concentration naphthalene system. This indicates that the adsorption of anthracene molecules to the soil surface is weaker, hence their diffusion capability in the aqueous medium is stronger.

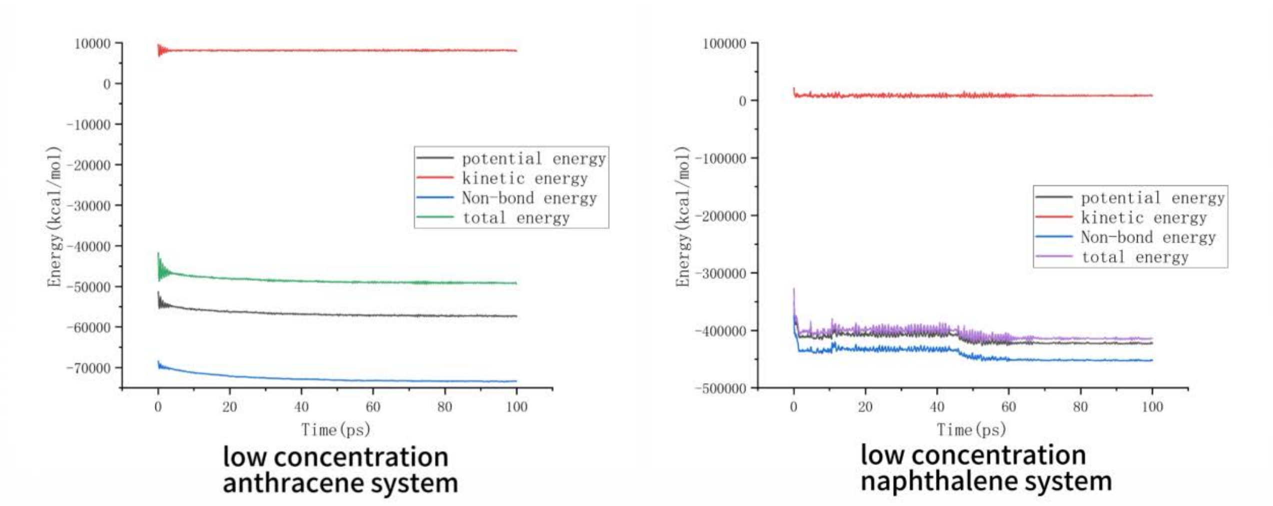

Figure 3: Energy Change Graph of Different Pollutants at Low Concentration

Furthermore, from Figure 4 which shows the mean square displacement (MSD) graph of different pollutants at low concentrations, significant differences in MSD values can be observed between anthracene and naphthalene on the SiO_2 surface, with anthracene having a larger MSD value than naphthalene. In summary, under low concentration conditions, naphthalene molecules have a more significant potential impact on soil, while anthracene molecules tend to diffuse more in the aqueous environment.

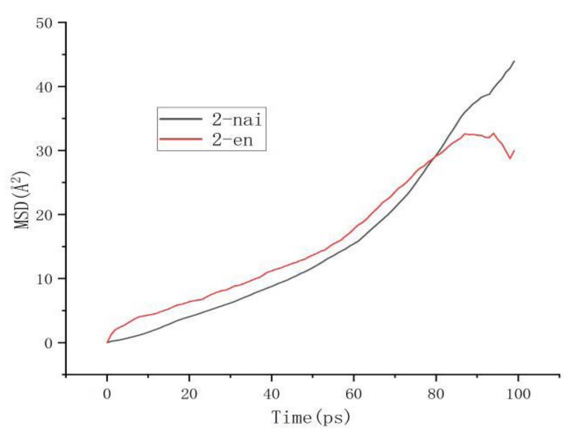

Figure 4: Mean Square Displacement of Different Pollutants at Low Concentration

3.2 The impact of different pollutants on soil water at high concentrations

In Figure 5, snapshots of the model structures of different pollutants at high concentrations are shown. It is observed that naphthalene molecules have a greater degree of diffusion in water, a phenomenon mainly due to the higher molecular weight of naphthalene molecules compared to anthracene molecules. In high concentration systems, the difference in molecular mass becomes more pronounced, and under the influence of gravity, molecules with larger molecular weights are more mobile, thus naphthalene molecules exhibit stronger diffusion capabilities.

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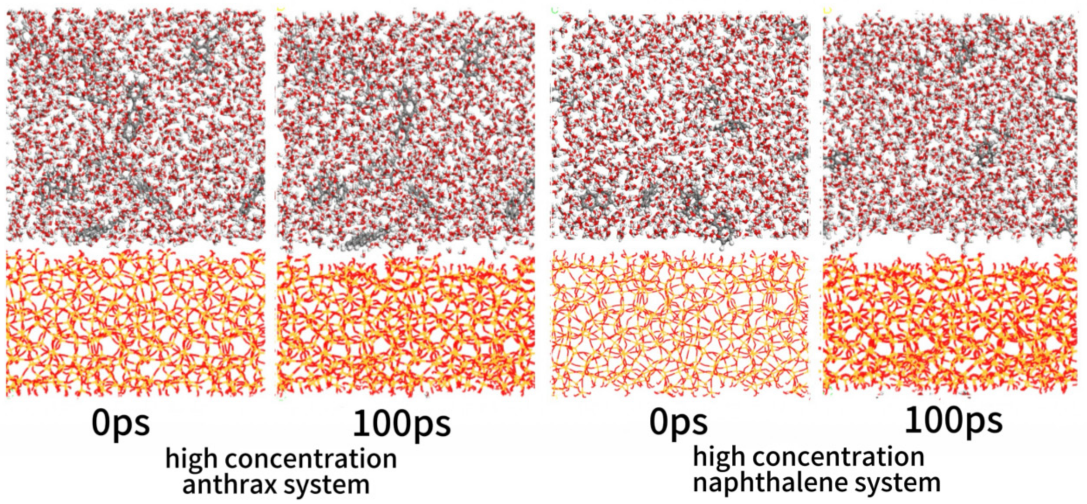

Figure 5: Snapshots of Model Structures of Different Pollutants at High Concentration

By monitoring the energy changes in the system, as shown in Figure 6 which illustrates the energy change graph of different pollutants at high concentrations, we can gain a deeper understanding of the interaction between pollutants and the SiO_2 surface. Data indicates that In the high-concentration naphthalene system, the potential energy continues to decrease, which indicates that under the action of gravity,the naphthalene molecules continue to diffuse, resulting in a decrease in potential energy. This shows that the naphthalene molecule is more likely to diffuse in water at high concentrations. On the contrary, in the high-concentration anthracene system, the potential energy is stable, suggesting that the anthracene molecule is more stable in the soil.

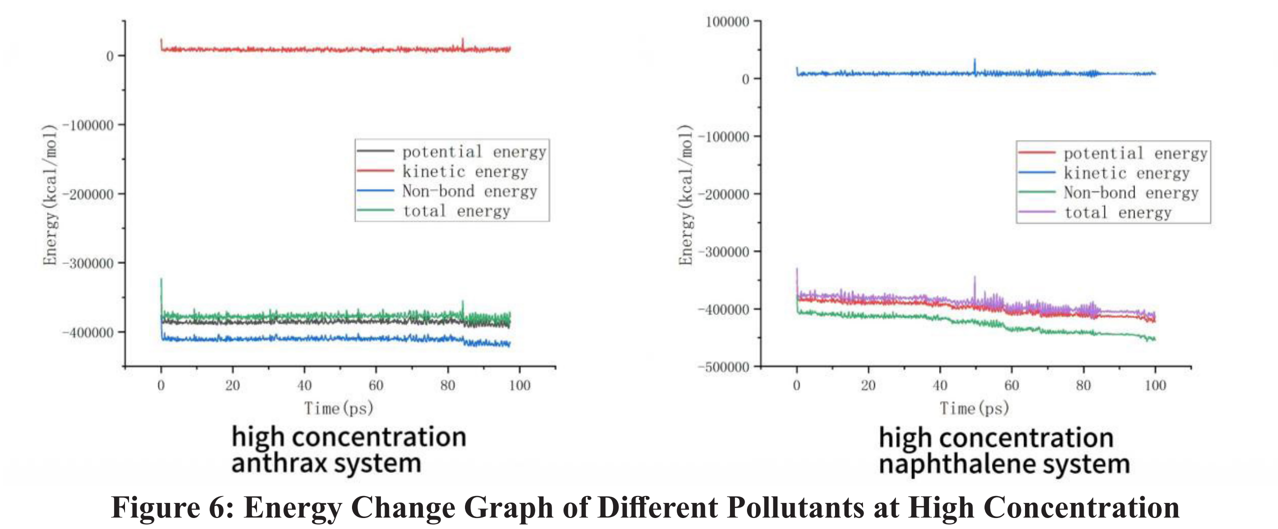

Figure 6: Energy Change Graph of Different Pollutants at High Concentration

Besides this, in Figure 7 which shows at high concentrations the mean square displacement (MSD) graph of different pollutants, significant differences in MSD values can be observed between anthracene and naphthalene on the SiO_2 surface, with naphthalene having a higher MSD value than anthracene. To sum up, at high concentration conditions, anthracene molecules have a more significant potential impact on soil, while naphthalene molecules tend to diffuse more in the aqueous environment.

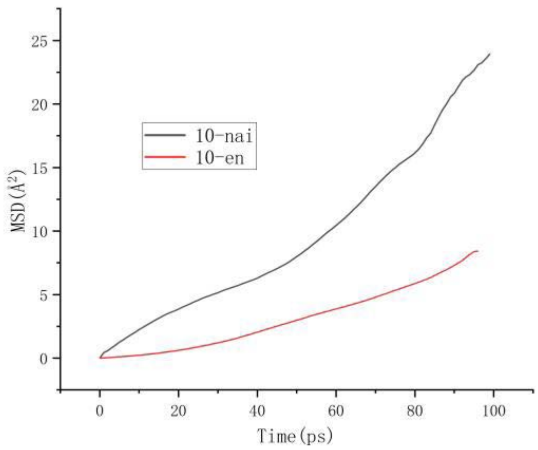

Figure 7: Mean Square Displacement of Different Pollutants at High Concentration

3.3 The impact of mixed pollutants on soil water

Both naphthalene and anthracene, are present in the solution at the initial moment, while the naphthalene molecules tend to adsorb behave under the surface of the material at the termination time. By analyzing the adsorption characteristics of the soil for molecules of different molecular weights, it is found that the soil has a stronger adsorption effect on larger molecules. In the situation of coexistence of mixed pollutants, compared to anthracene molecules, naphthalene molecules show a higher tendency to adsorb on the soil surface.

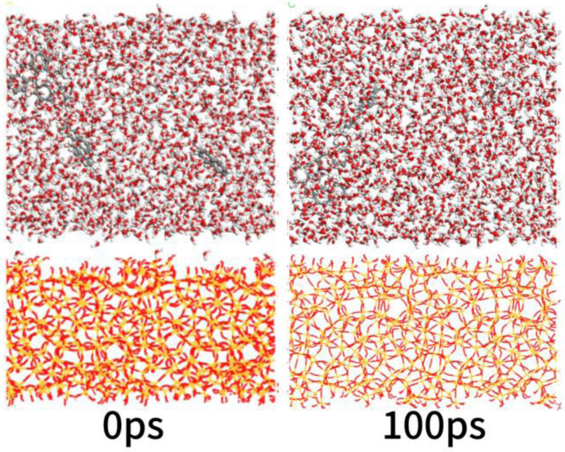

Figure 8: Snapshots of Model Structures of Different Pollutants in Mixed Systems

The results show that in mixed systems, a competitive adsorption phenomenon is observed between naphthalene and anthracene, leading to the instability of the soil surface's adsorption capacity for pollutants. In environments with multiple pollutants, the adsorption selectivity of the soil surface for organic pollutants may change.By analyzing the mean square displacement of anthracene and naphthalene molecules, we found that before 50 picoseconds (ps), there weren't significant differences in the MSD values of both, indicating that at the initial stage, the diffusion behavior of both molecules in the solution was similar. However, after 50 ps, the diffusion rate of naphthalene exceeded that of anthracene, which reviews in the mixed system, naphthalene molecules began to diffuse from the soil surface into the water during the competitive adsorption process with anthracene molecules. Additionally, at the 50 ps mark in the mixed system, we observed a transient decrease in energy. This phenomenon may be due to competitive adsorption, which leads to energy redistribution of the system.

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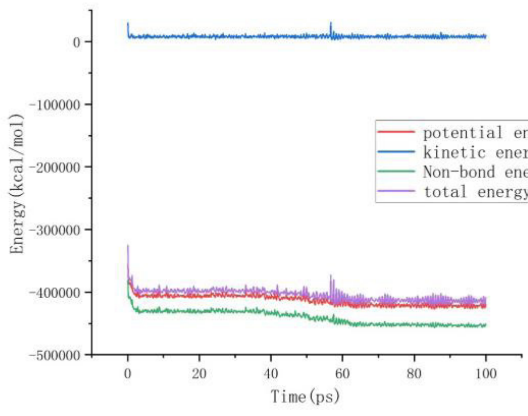

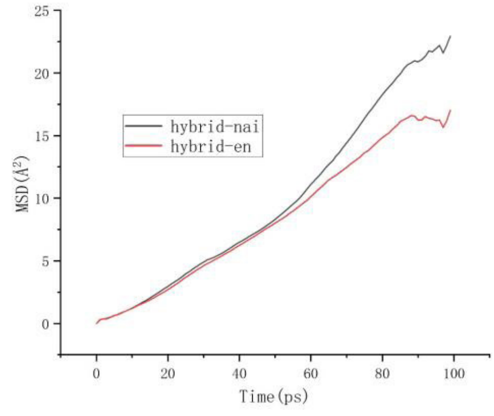

Figure 9: Energy Change Graph of Pollutants in Mixed Systems

Figure 10: Pollutants'Mean Square Displacement in Mixed Systems

In conclusion, this paper demonstrates that in a mixed system, the competitive adsorption phenomenon significantly affects the adsorption selectivity of the soil surface for different organic pollutant molecules. This competitive adsorption not only alters the adsorption stability of pollutants on the soil surface but may have a significant impact on the migration and transformation of pollutants in the environment.

4. Conclusion

In this paper, through molecular dynamics simulation methods, this study conducted an in-depth analysis of the diffusive behavior of aqueous and organic pollutants within the soil environment. The results reveal that at low concentration conditions, anthracene molecules exhibit stronger diffusion ability due to lower molecular weight; while under high concentration conditions, naphthalene molecules have stronger diffusion capabilities due to their larger molecular weight. Apart from this, competitive adsorption in mixed pollutant systems significantly affects the adsorptive selectivity towards various organic pollutant molecules on soil surfaces. With changing the adsorptive stability of pollutants on the soil surface, may exert a substantial impact on the migration and transformation of pollutants in the environment. These findings are of substantial significance for comprehending the transmission mechanism of pollutants in soil, predicting the diffusion process of pollutants, and formulating environmental protection measures. Future research could further explore the diffusion behavior of pollutants under different environmental conditions, as well as develop new soil remediation technologies to promote the healthy development of organic agriculture and environmental protection. Organic food is increasingly valued for its health and environmental benefits. However, the practice of organic agriculture has also brought a series of challenges, especially the issue of soil safety. Soil is the foundation of agricultural production, and its quality direct.

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