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Retraction

Retracted: Research Progress of Polycyclic Aromatic Hydrocarbons Pretreatment Methods and Application of Computer Simulation Technology for Prediction and Degradation of Electrochemical Concentration Detection

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This article has been retracted by Hindawi following an investigation undertaken by the publisher [1]. This investigation has uncovered evidence of one or more of the following indicators of systematic manipulation of the publication process:

(1) Discrepancies in scope
(2) Discrepancies in the description of the research reported
(3) Discrepancies between the availability of data and the research described
(4) Inappropriate citations
(5) Incoherent, meaningless and/or irrelevant content included in the article
(6) Peer-review manipulation

The presence of these indicators undermines our confidence in the integrity of the article's content and we cannot, therefore, vouch for its reliability. Please note that this notice is intended solely to alert readers that the content of this article is unreliable. We have not investigated whether authors were aware of or involved in the systematic manipulation of the publication process.

Wiley and Hindawi regrets that the usual quality checks did not identify these issues before publication and have since put additional measures in place to safeguard research integrity.

We wish to credit our own Research Integrity and Research Publishing teams and anonymous and named external researchers and research integrity experts for contributing to this investigation.

The corresponding author, as the representative of all authors, has been given the opportunity to register their agreement or disagreement to this retraction. We have kept a record of any response received.

References

[1] H. Chang and Y. Lu, "Research Progress of Polycyclic Aromatic Hydrocarbons Pretreatment Methods and Application of Computer Simulation Technology for Prediction and Degradation of Electrochemical Concentration Detection," *Journal of Chemistry*, vol. 2022, Article ID 6288072, 16 pages, 2022.

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Research Article

Research Progress of Polycyclic Aromatic Hydrocarbons Pretreatment Methods and Application of Computer Simulation Technology for Prediction and Degradation of Electrochemical Concentration Detection

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Polycyclic aromatic hydrocarbons (PAHs) are a class of organic compounds that are composed of aromatic rings containing only carbon and hydrogen atoms. They are one of the widespread environmental pollutants in the world. In recent years, many scholars have focused on the inhibition, formation mechanism, content of active components, and biodegradation effect of polycyclic aromatic hydrocarbons. They summarized the research progress of pretreatment methods for detection, but rarely discussed the experimental dataset for comprehensive analysis of pollution sources and the impact of different pretreatment technologies on the extraction of different substrates. What is more, computer simulation has not been mentioned. In this study, the pollution sources of polycyclic aromatic hydrocarbons (PAHs) are reviewed, and the related applications of various pretreatment methods such as gel permeation chromatography (GPC) are summarized. Finally, the computer simulation of the response surface method is introduced. The concentration of polycyclic aromatic hydrocarbons is tested or predicted by combining the neural network with the alternating trilinear decomposition (ATLD) algorithm, artificial population algorithm (ABC), and hierarchical genetic algorithm (HGA). Its future development trend is discussed and prospected, which provides a reference for solving the pollution problem. We look forward to providing help for the follow-up research of scholars in this field.

1. Introduction

There are two main sources of PAHs. The first is the natural source, mainly from the green vegetation of natural fire, volcanic eruption sediments, aquatic and terrestrial plants, and biosynthesis. The second is the man-made sources, mainly from incomplete combustion of coal, oil, natural gas and other fossil fuels, industrial processing, wood, traffic emissions, and road dust.

Among more than 100 kinds of polycyclic aromatic hydrocarbons (PAHs) that have been discovered and detected in nature, 16 PAHs have been listed as "priority pollutants under control" by EPA and the European Union. The nature and form of carcinogenic compounds cause a variety of degradation products that widely exist in the atmosphere, soil, and other environment, thus causing a wide variety of food or supplies such as dairy products, meat, seafood, nuts, and other pollution, which can be listed as one of the important pollutants. They will not only cause harm to ecological environment but also will pose a threat to human health.

In recent years, many scholars have summarized and discussed the inhibition, formation mechanism, content of active components, and biodegradation effect. There are few detection pretreatment methods to summarize the research progress, but these methods are not perfect. The impact of pollution sources and different substrates extracted by different pretreatment technologies on experimental data has been intensively analyzed, but computer simulation has rarely been mentioned and applied. In this study, the domestic and foreign literature on high temperature oil fume baked food, food packaging materials, atmospheric environment, water contact separation, detection, and extraction of polycyclic aromatic hydrocarbons in recent years were reviewed. Besides, their pretreatment was studied. This study reviews the research progress of correlation analysis technology in instrumental testing experiments and discusses and prospects the computer simulation of the response surface method and the application of the neural network in polycyclic aromatic hydrocarbons extraction. Besides, the future development trend of polycyclic aromatic hydrocarbons is discussed and prospected, which will be helpful to the research work of the scholars in this field.

2. Sources of Contamination by Polycyclic Aromatic Hydrocarbons

2.1. Contamination of High Temperature Smoked Food. Many studies have shown that barbecue and smoked foods in the process of production may induce the formation of polycyclic aromatic hydrocarbons. In particular, a certain amount of polycyclic aromatic hydrocarbons may be contained or produced in the pyrolysis of adipose tissue, incomplete combustion, high temperature fuming, and thermal polymerization of food fats; these will result in some residue on the surface of the food. Fasano and others found that when the temperature of the smoked products was higher than 200°, polycyclic aromatic compounds were produced and gradually migrated from the casing to the interior of the smoked products [1]. Chen and others studied and measured the content of PAHs in the smoke generated by heating model lipids and edible lipids; they found that PAHs and their derivatives were produced in the smoke generated by heating model lipids, and the content of the latter was significantly higher than that of the former [2]. Merlo and others analyzed five kinds of smoked bacon meats on the market and found that trace PAHs carcinogens were produced in the process of wood heating and the preparation of smoked bacon samples [3]. Shen and others found that during the smoking process, PAHs would be adsorbed on the meat surface in gaseous form or attached to the meat surface as particles. When the smoking process continues, PAHs that remain on the surface will penetrate into the internal part of the meat [4]. Kafouris and others analyzed PAHs in char-roasted pork and poultry, smoked pork, smoked hams, smoked sausages, and bacon. They found that 96% of the samples were contaminated with at least one PAH. Among these contaminated samples, 12% of the smoked products and 15% of the roasted meat samples exceeded the maximum level of EU legislation [5].

2.2. Contamination of Food Packaging Materials. In recent years, the safety of food packaging material has been greatly improved. More PAHs may be introduced into food packaging materials (such as impure paraffin oil) during the process of fluorescent whitening, bleaching, printing, printing, and waxing, thus affecting their safety [6]. Studies have shown that the use of food packaging contact materials contaminated with PAHs may lead to the spread of paHs to food, resulting in the contamination of packaged food. Therefore, the food industry should of course avoid improper use of packaging in the food production process. Moreover, the polluted plastic packaging materials should be processed centrally to prevent their indirect pollution to the natural environment [7]. Conchione and others were the first to investigate the presence of PAHs in pizza boxes containing recycled fibers and to assess the potential migration by conducting migration tests using the Tenax® animitator. The results showed that the high content of PAHs in the samples, especially chrysene, confirmed the migration potential of these pollutants [8]. Li and others detected eight kinds of PAHs in 21 samples of polystyrene food contact materials and evaluated the migration of PAHs by using the stochastic migration model. It was concluded that the migration rate of PAHs depends on the molecular structure and agglomeration properties of plastic materials [9].

2.3. Atmospheric Pollution. The PAHs mixture in the air is mainly accompanied by coal tar, automobile exhaust, and smoking smoke. In particular, the occurrence of haze is often characterized by a sharp increase in the concentration of particulate matter, which not only pollutes the natural environment such as agricultural products and soil but also causes great trouble to human production and life, as well as poses a great threat to human health. In addition, PAHs are also important organic components of environmental particulate matter (PM2.5) with diameter less than 2.5 microns. Among PAHs' derivatives, PAHs and hydroxyl PAHs have been detected in high concentrations of PM2.5 samples. It is an important way to enter the human lungs. He and others found in their studies that persistent organic pollutants (pops) such as polycyclic aromatic hydrocarbons (PAHs) in suspended particulate matter in the atmosphere will have a coupling effect with harmful algal blooms in the aquatic environment, thus causing pollution to lake water environment [10]. From September 2012 to August 2013 in China, Japan, South Korea, and other five Asian countries, Hong and others measured the concentrations of 47 kinds of PAHs in 176 sites in different seasons for four consecutive months, all of which were detected [11]. When studying the polycyclic aromatic hydrocarbons, Baek and others found that its concentration change has certain law in the spatial and seasonal distribution.

The polycyclic aromatic hydrocarbons' content shows obvious seasonal variation and the highest content appears in winter, so they concluded that the factors affecting the concentration of polycyclic aromatic hydrocarbons may have a direct relationship with home heating, fuel combustion in automobile exhaust, and industrial activity in its pollution sources [12]. Ma and others described 16 kinds of PAHs and 16 kinds of nitropolycyclic aromatic hydrocarbons (NPAHs) combined with inhalable particles in cold areas of China and analyzed their sources and health risks. They proposed that the main source of PAHs is combustion, and controlling the combustion of coal and biomass would be an effective measure to improve the air quality in Harbin during the heating period. And in addition to the direct emissions, about 20% of polycyclic aromatic hydrocarbons are from the second generation. According to the weather conditions on the influence of polycyclic aromatic hydrocarbons and unsaturated fatty acid concentration, it can be found that in the heating period, PAHs pollutants are more vulnerable to the influence of meteorological condition than in the non-heating period. The highest health risks caused by contacting PM10-PM2.5 with polycyclic aromatic hydrocarbons are also prone to happen in the winter. Health risk assessments have shown that there is a potential cancer risk associated with prolonged exposure to such environments [13].

2.4. Water Pollution. Studies have shown that organic pollutants such as PAHs exist in all kinds of aquatic systems, trace residues in sewage treatment plant inlet and outlet water, groundwater, surface water or seawater, and other water bodies [14]. Although the content is very low, it will have an impact on the natural environment and human health due to its persistence and accumulation. Chen Jiang et al. detected PAHs in mine drainage and underground water collected from many places. After analysis, they found the enrichment reason might be that PAHs and others organic substances are not easy to photodegradation in the dark and closed underground environment and are not easy to pyrolysis due to the constant underground temperature. In addition, some pollutants, including them, may be accumulated by the adsorption of deposits, coal, and rocks in the mine [15]. Ambade and others detected a trace amount of 16 PAHs in drinking water samples. After analyzing the physical and chemical parameters of all the samples, they believed that the pollution might be caused by the surface water pollution caused by industrial and domestic wastewater discharge, the precipitation and deposition of combustion sources, and the infiltration of PAHs from surface water sources to groundwater [16].

From the above analysis, it is not difficult to find that the pollution problem of PAHs is affecting our daily life, and the consequences will be hard to imagine if it is not controlled. However, with the rapid development of science and technology, the application of computer has gradually expanded up to a domain, represented by deep learning and machine learning. Cooperation with the relevant learning algorithm in compound properties prediction and treatment showed a better ability to frequently predict the simulation of various compounds in the experiments. In particular, the application of the artificial neural network in chemical analysis and other fields has emerged, which not only avoids repeated and redundant experimental operations but also saves experimental operation costs and effectively improves work efficiency. In addition, the computational simulation method can also describe the adsorption separation process at the microscopic level, which cannot be replaced by experiments. In this study, response surface methodology and neural network are reviewed. It is not difficult to find that it is very important to choose appropriate pretreatment technology and detection method for further effective monitoring of PAHs. In this study, through a large number of literature reviews, this study compares and summarizes several commonly used new pretreatment application technologies. Advantages, disadvantages, and adaptability are integrated to make a comprehensive and systematic review.

3. New Pretreatment Application Technology for Polycyclic Aromatic Hydrocarbons Concentration Detection

3.1. Gel Permeation Chromatography (GPC). Gel permeation chromatography (GPC), as one of many new separation technologies, is mainly used in the detection of multi-pollutant residues in agricultural residues, food, and oil and has been applied to the detection of polycyclic aromatic hydrocarbons. In the determination and analysis of PAHs in edible oil samples, Wang and others [17] used gel permeation chromatography to remove triglycerides in the samples before treatment. Lian and others [18] used gel permeation chromatography to reduce matrix interference in the pretreatment of determination of 16 PAHs in cigarette samples, which can obtain cleaner final extract than traditional solid-phase extraction technology, making the analysis results more accurate and ensuring reliable routine determination at a low level. Shao and others [19] took agricultural land in the suburbs of Tianjin as the research object to analyze the content of 16 kinds of PAHs in typical soil samples and purified them by gel permeation chromatography and other technologies before treatment. Through analysis, it is found that some sites near the city are seriously polluted by polycyclic aromatic hydrocarbons. Coal burning is still the main pollution source in Tianjin. Data from the experiment can be further used to assess the health risks associated with PAH-contaminated soils and help local governments find appropriate ways to reduce PAH-contaminated soils; Kong and others [20] used gel permeation chromatography to purify samples in the pretreatment experiment of 15 PAHs in the determination of adipose tissue, and the determination results met the verification criteria.

It can be seen from the above examples that gel permeation chromatography, as a pretreatment technology, is often combined with GAS chromatography-tandem mass spectrometry to detect PAHs in the matrix, which effectively avoids the volatilization of reagents, and has the advantages of strong resistance to matrix interference and high sensitivity. Besides, it can be continuously and automatically analyzed to improve the accuracy of results. It can also be seen from Table 1 that the average recovery rate of samples is at a high level, and other coefficients are within the standard range. Therefore, gel permeation chromatography can be used for purification when the extracted PAHs samples contain lipids, pigments, alkaloids, polymers, and other pretreatment methods.

3.2. Molecular Imprinting (MIP). Molecular imprinting (MIP) technology, which is based on simulating the interaction between receptors and antibodies in nature to prepare

Table 1: Effect of gel permeation chromatography on the determination of polycyclic aromatic hydrocarbon in different substrates.

Substrate	Method	LOD (μg/kg)	Recovery (%)	R^2	RSD (%)	References
Oil	UHPLC-DAD-FLD	0.0025–0.01	73–110	>0.999	<10	[17]
Cigarette	GC-MS	0.1–0.8	83–104	*	<10	[18]
Soil	GC-MS	0.16–9.36	64.6–111.9	0.99 (B [a] p)	1.3–16.5	[19]
Fat	GC-MS	0.1–6.6	120–130	≥0.99	8.48–20.3	[20]

molecularly imprinted polymers with specific selectivity for specific target molecules, has obvious advantages especially in the trace analysis of complex matrix samples in the fields of food safety, environmental, and pharmaceutical analysis. Known as the manufacture of "molecular key" "artificial lock" technology, more and more attention are given at home and abroad. In addition, molecularly imprinted SPE column can be reused, and the experimental cost can be saved because of its resistance to strong acid and alkali and other adverse environmental damage. Rajendran et al. [21] selected four biological samples from cereals, animals, and humans as representative lipids to explore the potential application of MIP adsorbent in the analysis of PAHs in lipid matrix biological samples. They compared it with the commonly used gel permeation chromatography. The results show that MIP can be used for the analysis of PAHs in biological samples of various lipid substrates. Compared with the traditional GPC method, the MIP method has less experimental time and solvent consumption. In addition, the recovery rate of 16 PAHs homologues by the MIP method is similar to that by the GPC method. The results show that the MIP method can be used as an alternative method for the analysis of PAHs in biological samples with various lipid substrates (Figure 1). Geiss et al. [22] developed a simple, rapid, and economical method for the determination of eight preferred PAHs in rubber and plastic materials, which can improve extraction and cleaning procedures. The purification performance of silica gel packed column and MIPs solid-phase extraction column was qualitatively evaluated, and the superiority of solid-phase extraction based on MIP compared with the traditional silicification purification method was emphasized. Combined with gas chromatography-mass spectrometry (GC-MS) analysis of selective ion mode, it was found that the method had high extraction efficiency, purity, and speed. Zhou et al. [23] proposed a novel purification method based on the combination of molecularly imprinted polymer (MIP) and polycyclic aromatic hydrocarbons (PAHs) to determine 24 PAHs in edible oil. Under the optimized conditions, the coefficient indexes are good. Krupadam et al. [24] selected molecular-imprinted poly (vinylpyridine-co-ethylene glycol dimethacrylate) as the experimental pretreated solid-phase extraction material to determine five carcinogenic polycyclic aromatic hydrocarbons in atmospheric dust, which is easy to operate and has high stability. In addition, organic matter in air dust has no influence on MIP extraction, which can be used for trace determination.

By comparing the data in Table 2, it was found that the detection method for PAHs was mostly gas chromatography-mass spectrometry (GC-MS) when molecularly imprinted solid-phase extraction (MISPE) was applied. The sample recovery was also at a high level with good parameters. The technique is formed by the copolymerization of cross-linked monomers, which can absorb specific PAHs through noncovalent interactions, allowing rapid, accurate, and highly selective extraction of target analytes from complex matrices during preprocessing of samples. It can be used in the selective determination of pesticide residues, drugs, organic dyes, mycotoxins, and persistent organic pollutants in food substrates in the pretreatment of samples. Through reading the above literature, it can be found that the molecularly imprinted solid-phase extraction method is similar to the GPC method in terms of impurity removal, polycyclic aromatic hydrocarbon recovery, total cost of materials, and reagents. However, Sun and others found in the experiment that some impurities could not be completely removed by using the GPC method. Therefore, molecularly imprinted technology is more appropriate to protect the GC-MS system. In addition, this method can process samples in batches, while the GPC method can only process one sample at a time, and MIP technology can avoid excessive time consumption.

3.3. Accelerated Solvent Extraction (ASE). Accelerated solvent extraction (ASE) has been widely applied in many fields, which has the characteristics of less solvent, high selectivity, high extraction efficiency, and simplified operation steps. Zhang and others [25] used a combination of rapid solvent extraction and solid-phase extraction to determine the content of seven polycyclic aromatic hydrocarbons (PAHs) in soil and earthworm samples for sample pretreatment, then purified by solid-phase extraction column, and evaporated by a rotary evaporator to dry. This method has high recovery rate and good reproducibility and can be used for quantitative analysis of PAHs in soil and earthworm samples. Dinović-Stojanović and others [26] verified the detection methods of several PAHs in smoked meat products. The accelerated solvent extraction method and solid-phase extraction method were used for further purification of target substances. Experimental results showed that this method could be used for the analysis and detection of several PAHs in smoked meat products. Suranová and others [27] used accelerated solvent extraction equipment such as separation and extraction and presmoked meat samples in lipid compounds and oily impurity such as interference. The method is simple to operate, and the recovery rate is in line with relevant standards. The applicability of the method is verified on the final food analysis performance evaluation program certification material (smoked meat products), and the data results are consistent;

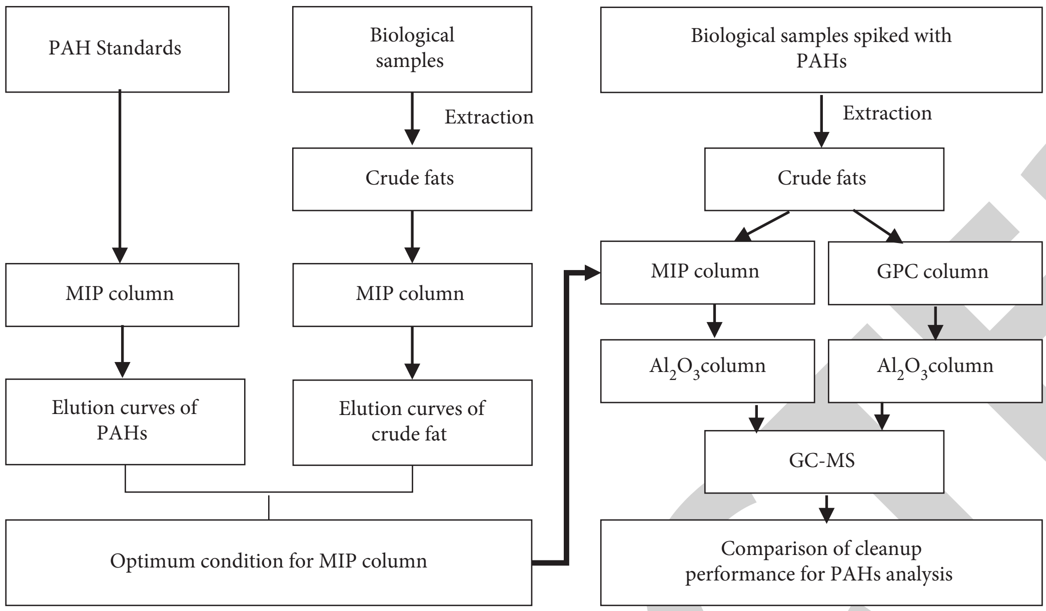

Figure 1: The schematic flowchart of the experimental design.

Table 2: Effect of molecular imprinting-gas chromatography on the determination of polycyclic aromatic hydrocarbon in different substrates.

Substrate	Method	LOD (μg/kg)	Recovery (%)	R^2	RSD (%)	References
Biological sample	GC-MS	*	75–120	*	*	[21]
Rubber plastic material	GC-MS	*	79–99	>0.99	1.4–10.8	[22]
Oil	GC-MS	0.1–1.0	86–116	≥0.9990	≤10.8	[23]
Atmospheric dust	GC-MS	0.5–0.9	5–97	0.998	1.8–2.7	[24]

Tan and others [28] determined polycyclic aromatic compounds such as phenanthrene, pyrene, and acenaphthene in fish by stable isotope dilution gas chromatography-tandem mass spectrometry and extracted fish samples by an improved accelerated solvent extraction method to eliminate the influence of potential matrix interference. The results showed that the method met all the standards stipulated by the European Commission legislation.

After reading the above literature, it is found that rapid solvent extraction technology is a technology with higher extraction rate than traditional solvent. By increasing the temperature and pressure, the solvent is in liquid form, which accelerates the extraction power of solvent, improves the extraction efficiency of sample, and reduces the extraction time and reagent of target substance. Due to the semivolatile and nonvolatile characteristics of PAHs, rapid solvent extraction technology can be selected as the sample pretreatment technology.

It should be noted that this kind of pretreatment technology has high requirements for testing instruments, and the extraction agent, eluent, and volume ratio also have a certain influence on experimental results. It is mainly used for testing the residues of polycyclic aromatic hydrocarbons and pesticides in food in physical and chemical testing. As can be seen from Table 3, the rapid solvent extraction method is mostly used in combination with the high performance liquid chromatography-fluorescence detection method, and the linear relationship coefficients are all at a high level.

3.4. Matrix Solid-Phase Dispersion Extraction (MSPD). Matrix solid-phase dispersion (MSPD) is used to fully mix the sample and adsorbent and grind it into a semisolid column for elution. MSPD has the functions of dispersion, extraction, and purification and has the characteristics of simple and quick operation and strong resistance to matrix interference. So far, MSPD has been widely used in the analysis of various compounds in various matrices. Sharma et al. [29] established a rapid method for simultaneous determination of 4 PAHs in bovine tissues. The matrix solid-phase dispersion technique was used to collect samples from the bovine muscle, liver, and lung that died of free pathological injury, and the results of various parameters obtained were within the standard range. Liu et al. [30] analyzed and determined 16 kinds of PAHs in soil samples by using matrix solid-phase dispersion technology to purify and elution soil samples, eliminating most of the interfering matrix components. In order to obtain a higher recovery rate, the results show that the method can be used for soil PAHs analysis and save the solvent consumption, material cost, sample operation, and required time. When analyzing polycyclic aromatic hydrocarbons (PAHs) in fish tissues, Huang et al. [31] used matrix solid-phase dispersion technology to treat

Table 3: Effect of accelerated solvent extraction chromatography on the determination of polycyclic aromatic hydrocarbon in different substrates.

Substrate	Method	Extraction solvent (v/v)	Eluent (v/v)	LOD (μg/kg)	Recovery (%)	R^2	RSD (%)	References
Soil earthworm	HPLC-FLD	N-Hexane-O-acetone (4 : 1)	N-Hexane-dichloromethane (9 : 1)	0.15–0.85	83.5–110.2 (soil); 81.2–97.1 (earthworm)	0.9998–1.000	1.1–4.6 (soil); 1.6–4.2 (earthworm)	[25]
Smoked meat	HPLC-FLD	N-Hexane (*)	N-Hexane (*)	0.03–0.2	>96.3	0.993–0.997	*	[26]
Smoked product	HPLC-FLD	Acetone-n-hexane (*)	Acetone-n-hexane (*)	5 0.11–0.23	74 ± 7–109 ± 11	0.99988–0.9999	4.4–11.6	[27]
Fish	GC-MS	Dichloromethane-n-hexane (4 : 1)	Dichloromethane-n-hexane (4 : 1)	0.06–2.28	44.8–133.7	0.9968–0.9998	3.1–9.6	[28]

Table 4: Effect of the matrix solid-phase dispersion method on the determination of polycyclic aromatic hydrocarbon in different substrates.

Substrate	Method	Dispersant	Substrate: dispersant	Eluent	LOD (ng/g)	Recovery (%)	R^2	RSD (%)	References
Cattle tissues	HPLC-FLD	C_{18}	4 : 1	Acetonitrile + water	0.012	96.4–98.8	0.998	≤10	[29]
Soil	HPLC-FLD	Florisil® + SiO_2	2 : 1 : 1	Acetone + hexane	0.01–0.6	94.3–103.9	0.9996	0.6–1.9	[30]
Fish tissue	HPLC-FLD	Florisil + C_{18} + Na_2SO_4	6 : 10 : 20 : 5	Hexane + dichloromethane	0.04–0.32	80.4–105.4	*	2.14–7.87	[31]
Microbial culture solution	HPLC-FLD	C_{18}	1 : 20	Acetonitrile + water	0.02–0.03	>90	>0.99	3.6–4.1	[32]

samples and investigated the suitability of different solid carriers and their influence on the extraction efficiency of natural fat content in samples. The reproducibility of the experimental results is good, and the detection and quantification limits are far below the maximum allowable levels stipulated by European Union and national regulations. Therefore, MSPD can be used as a good alternative method to extract PAHs from fish tissues in the pretreatment experiment. Llasera and others [32] used the high performance liquid chromatography and fluorescence detection method to quantitatively detect PAHs in microbial liquid culture of ciliate protozoa. Since there are few analytes extracted from microorganisms and insoluble organics in the sample, the MSPD method is selected for pretreatment (Table 4).

After reading the above literature, it can be found that the matrix solid-phase dispersion method can integrate the process of sample crushing, homogenization, extraction, purification, and separation into one step, which is green, simple, and efficient. The advantages of this method are reflected in the consumption of samples and organic solvents, environmental protection, experimental cost, simplicity of extraction process, and time consuming. In addition, there is no need to use ultrasonic, microwave, and other auxiliary extraction methods, without heating, so as to avoid the degradation of the target analyte.

Second, if this method is used to obtain the maximum extraction efficiency of the target component, the molecular structure of the target analyte, the type of dispersant elution solvent, and the volume ratio should be taken into account. Experimental selection should be optimized; the obtained linear relationship detection limit precision stability recovery data should also be integrated in the form of tables.

In addition, it was found that in the extraction of PAHs, if the matrix components are complex, gel permeation chromatography, rapid solvent extraction, pressurized solvent extraction, and solid-phase extraction (SPE) may be needed to assist purification, so as to establish a new method of dispersed matrix SPE. In summary, MSPD can be considered as the purification method if the plan is to extract PAHs from complex solid and semisolid samples such as insoluble lipophilic substances and organic matter.

3.5. Magnetic Solid-Phase Extraction (MSPE). Magnetic solid-phase extraction (MSPE) technology is to select a specific magnetic or magnetized material as the adsorbent, through the effect of magnetic field to separate the sample from the matrix, in addition, considering that there may be a small amount of sample residue on the magnetic adsorbent, so the final need to elute it, to get more accurate results. Qin et al. [33] chose Fe_3O_4@PDA@PCD as the adsorbent and used magnetic solid-phase extraction to analyze 6 PAHs in soil. When the adsorption efficiency of Fe_3O_4@PDA@PCD and Tenax resin is 90%, the time required for PAHs to reach adsorption equilibrium is compared. It is found that Fe_3O_4@PDA@PCD (5 min) is much smaller than Tenax resin (30 min). Compared with the latter, the former has higher dispersion in aqueous solution, so it takes less time to reach adsorption equilibrium. The MSPE method was used to determine the cumulative concentration of PAHs in

Table 5: Effect of magnetic solid-phase extraction on the determination of polycyclic aromatic hydrocarbon in different substrates.

Substrate	Method	Adsorbent	Adsorption equilibrium time	Recovery (%)	R^2	RSD (%)	LOD (μg/kg)	References
Soil	GC-MS	Fe_3O_4@PDA@PCD	5 min	86–98	$R^2 = 0.98$	<10	*	[33]
Milk product	GC-MS	MWCNT-MNP	5 min	>86.1	0.981–0.992	3.2–10.1	0.04–0.075	[34]
Water	HPLC-FLD	Fe_3O_4@SiO_2@MMTA-Au	90 s	87.8–120	0.9919–0.9985	1.14–3.45	0.25–37.5	[35]
Water	HPLC-FLD	Fe_3O_4@MIL-101	<30 min	*	0.9978–0.9992	3.3–4.8	*	[36]

earthworms, and the correlation analysis was conducted with the extracted amount. The applicability of the MSPE method in biological feasibility assessment earthworms proved that the method can be used to predict and analyze PAHs in soil. Nabi et al. [34] studied 16 kinds of PAHs in dairy products by MSPE/GC-MS and discussed the influence of different factors on the content of PAHs in different types of dairy products. MWCNT-MNP complex of CNTs surface modified by adsorbent was quantitatively analyzed by SIM. The results showed that the linear relationship of the method was good and the recovery rate was high. Except for few milk powder samples, the content of PAHs in other samples was lower than the EU standard limit. Yang et al. [35] prepared a new magnetic adsorbent and utilized the 90s magnetic solid-phase extraction method to complete the adsorption, which greatly saved the time of sample pretreatment. Li and others [36] chose to use metal-organic skeleton composite material (Fe_3O_4@MIL-101) as magnetic solid-phase extraction adsorbent to determine PAHs in tap water samples. They combined the high-performance liquid chromatography-fluorescence method for qualitative and quantitative analyses, avoiding cumbersome operations such as filtration and optimizing experimental operations.

Searching keywords “PAHs” and “MSPE” in Web of Science database, it can be found that in recent years, magnetic solid-phase extraction has been widely used in the determination and analysis of PAHs. Magnetic adsorbents were prepared according to the characteristics of extraction environment. Due to its unique discrete properties and the effect of external magnetic field, easy to operate, high efficiency, and green environmental protection, extraction efficiency is also considerable. In addition, the number of adsorbent cycles is also beneficial to reduce the cost of the experiment. In addition, through the analysis of the data given in Table 5, it can be seen that the standard recovery rate of the sample after the application of this technology is high, and the linear relationship and other parameters are in the standard range. In conclusion, as one of the most promising sample pretreatment technologies, magnetic solid-phase extraction (MSPE) will be applied more widely in food safety and other fields in the future.

3.6. Cloud Point Extraction (CPE). Cloud point extraction (CPE) is a green extraction technology based on the phenomenon of cloud point and the solubility of micelle solution to achieve the separation of water-soluble substances from hydrophilic or oily substances. Matsuura and others [37] used the turbidity point extraction method and selected Brij30 as a nonionic surfactant to separate phenanthocyanin from soil. In the experiment, the effect of two salt additives on promoting phase separation in CPE was investigated. It was found that the turbidity point temperature decreased by about 30°C with the addition of sodium chloride, while the turbidity point temperature decreased by about 45°C with the addition of sodium sulfate, so sodium sulfate was selected. In addition, the gravity sedimentation method was used to replace centrifugal separation in the separation of PAHs in the washing solution, so that a large number of samples could be processed at a lower cost. The experimental results show that the sample recovery rate is high, which also proves that the method is economical and effective for treating a large amount of contaminated soil. Soares and others [38] used turbidity point extraction and OPEO30 surfactant phase derivations and gas chromatography-mass spectrometry to detect PAHs in groundwater samples. According to the multiple response, Pareto diagram, curvature test and chromatographic data analysis, the experimental scheme was designed using central point experimental conditions and the optimal conditions were determined. The multiple response was calculated using the following equation:

$$\text{Multiple response} = \sum\left(\frac{\text{PAH area}}{\text{Maximum PAH area obtained in design}}\right). \quad (1)$$

Compared with LLE, this method has the main advantages of using nontoxic solvent in small volume and low volume samples and conforms to the principle of green chemistry. Jia et al. [39] established a turbidity point extraction method based on the hexafluoro-isopropanol (HFIP) mediated TX-100 water system. The results proved that the HFIP-mediated CPE enrichment factor and extraction rate were better. This method is simple, rapid, and reliable and can be used for the extraction and detection of polycyclic aromatic hydrocarbons organic pollutants in water.

Through the analysis of Table 6 content, it was found that the turbidity point extraction method could be used to detect trace PAHS pollutants in the pretreatment of food, water samples, and soil. The HPLC-UV method was mostly used for detection. Low toxicity and nonvolatile nonionic

Table 6: Influence of cloud point extraction on determination of polycyclic aromatic hydrocarbon in different substrates.

Substrate	Method	Surfactant	Temperature (°C)	Recovery (%)	LOD (μg/L)	References
Soil	HPLC-UV	Brij30	25	58–88	*	[37]
Water	GC-MS	OPEO30	70	70–98	0.02–0.05	[38]
Water	HPLC-UV	HFIP-TX-100	26	79.4–110.8	0.04–0.38	[39]

surfactants were widely used in the preconcentration process. Initiation initiates the separation of the aqueous phase close to the critical micelle concentration from the surfactant rich phase. In order to improve the extraction efficiency, the selection of surfactant is particularly important.

3.7. Other Technologies. Manzano et al. [40] used two-dimensional gas chromatography-time-of flight mass spectrometry to quantitatively analyze complex PAHs mixtures in NIST SRMs. High orthogonality column combination (LC50 × NSP-35) was used to quantify complex PAHs mixtures in NIST SRMs, achieving better chromatographic resolution and greater orthogonality. In addition, it can be used to accurately quantify complex PAHs mixtures in environmental extracts and comprehensively determine their complex PAHs composition. Ramos-Contreras and others [41] developed a green method based on pressurized hot water extraction (PHWE), micromembrane-assisted solvent extraction (MASE), and temperature programmed evaporation gas chromatography-ion trap tandem mass spectrometry (PTV-GC-MS/MS) for the analysis of 16 polycyclic aromatic hydrocarbons (PAHs) and 8 related compounds in atmospheric particulate matter. The critical water extraction-membrane microextraction method is proved to be reliable and effective for the determination of trace PAHs in atmospheric particulate matter. Cochran and Kubatova [42] proposed an effective method for simultaneous extraction of polycyclic aromatic hydrocarbons (PAHs) and their polar oxidation products from atmospheric particulate matter by pressurized fluid extraction (PFE).

In recent years, donor-acceptor complex chromatography (DACC) has been used for the detection of PAHs as a new technology, which can reduce the amount of solvent and save the analysis time in the purification of tested samples. Windal et al. [43] used donor-receptor complex chromatography (DACC) combined with high-performance liquid chromatography-ultraviolet/fluorescence detection to analyze 16 European priority PAHs in fish oil and dried plants, and the results showed that the detection of most of them showed good linear relationship. Barranco et al. [44] compared the purification method based on the donor-acceptor composite chromatography column (DACC) with the standardized method widely used in food industry (low-pressure column chromatography with alumina as the stationary phase) in the pretreatment analysis of polycyclic aromatic hydrocarbons (PAHs) in edible oil, and the results showed that DACC is used to control the type of mobile phase and the flow rate, which not only optimizes the pretreatment operation and saves the elution time but also cleans the sample, facilitates the follow-up detection, and makes the experimental results reach a more accurate and higher level.

4. Application of Computer Simulation in Concentration Detection, Prediction, and Degradation of Polycyclic Aromatic Hydrocarbons

4.1. The Response Surface Method. The response surface method first appeared in the 1950s. The history is not long, but it develops rapidly. It was proposed by Box and Hunter in 1951. Hill, Hunter, Draper, Khuri, Comell, and other scholars have conducted some preliminary application studies and preliminary definitions of response surface methodology successively and made a relatively comprehensive and systematic discussion.

In this method, the response surface model and function relationship are fitted by finite number of tests and test data. Through optimization calculation, the best combination of test variables and the best process parameters is found. In recent years, RSM has been widely used in food, Chinese medicine, engineering, ecology, biological engineering, and many other fields.

The prediction based on the RSM statistical model not only provides the best prediction for parameter optimization but also reduces a lot of laboratory work. Abd Manan and others used response surface methodology (RSM) to study the optimal conditions for photofenton oxidation to degrade polycyclic aromatic hydrocarbons in drinking water. The drinking water samples were prepared with an aqueous solution at a water treatment plant in Perak, Malaysia, in September 2016. The reaction time, pH value, and molar concentration of H_2O_2 and $FeSO_4$ were determined by the RSM method. The influences and interactions of these parameters were evaluated by using a five-stage central composite design of the quadratic model. The response variable was the total organic carbon (TOC) removal rate, and the quantitative analysis of polycyclic aromatic hydrocarbons was performed by gas chromatography-mass spectrometry [45]. Gitipour and others established a mathematical model with response surface methodology to quantify the influence of three parameters, including washing temperature, washing time, and detergent, on the washing process of PAH-contaminated soil. In the experiment, the DOE method was used to carry out 20 experiments to maximize the removal efficiency of PAHs by combining research variables. The three factors studied varied within a predetermined range, and the output (i.e., removal rate) was evaluated to compare the removal process of each PAH, so as to obtain the model of the total removal rate of PAHs and finally obtain the optimal conditions related to the parameters studied. In addition, the established secondary model for removing PAHs also has a high correlation coefficient [46]. Ramalhosa and others established a microwave-assisted extraction (MAE)-liquid chromatography-photodiodearray (LC-PDA) combined fluorescence detection method and used response surface methodology to find the optimal extraction parameters. They analyzed and determined 18 PAHs in the food tissues of three common edible and commercial fishes (sardines, mackerel, and horsemackerel) from the Atlantic Ocean. Different levels of naphthalene and other PAHs were detected in the samples analyzed, and none of the samples contained benzo [a] pyrene, a marker used to evaluate the occurrence and carcinogenesis of PAHs in food. The application of the RSM method can fully consider the possible interaction between variables, while avoiding the method of one-factor experiment. This method is sensitive, efficient, simple, and robust and can be used for routine analysis [47]. Gfrerer and others used the response surface design method to optimize the extraction of PAHs using the new process, taking the changes of extraction cycles and holding time after reaching the heating temperature as experimental variables. The comparison shows that fluidized bed extraction is an effective alternative method to extract PAHs from soil and sediment. The recoveries and relative standard deviations are in the acceptable range. The results provided by this method are similar to those of the standard Soxhlet extraction method. Compared with traditional methods, this method has the advantages of short extraction time, less solvent consumption, and higher efficiency and precision [48]. Hui et al. prepared poly-β-cyclodextrin ionic liquid FF using n-octanol as supramolecular solvent as a new extractant. In combination with GC-FID, the main variables of FF formation time (min), volume of SUPRAs (LAIRL), and extraction time (min) were optimized by variation-by-variable (OVAT) analysis and response surface methodology (RSM). It was successfully applied in dispersive liquid phase microextraction of seven representative PAHs. The application of magnetic separation avoids the traditional microextraction techniques such as centrifugation or filtration, which greatly improves the separation rate. OFAT analysis is used to screen and determine the variables that affect the extraction efficiency, and the optimized method has been successfully applied to the content safety study of polycyclic aromatic hydrocarbons in a variety of commercial food and beverage in Malaysia [49].

Central combination design based on the response surface method is an effective method to seek optimal conditions for multivariable systems. This method not only reduces the number of experiments and improves the possibility of statistical interpretation but also indicates whether the parameters interact. Lu et al. used a physiology-based method to simulate human digestion in vitro and analyzed the effects of soil/liquid ratio (S/L), pH value, and culture time on the bioacceptability of PAHs in simulated gastrointestinal soil using response surface methodology combined with the central composite design method [50]. Chen and others used response surface methodology designed by Box–Behnken to study the effects of substrate concentration, inoculation amount, and temperature on the degradation of polycyclic aromatic hydrocarbons (PAHs) in petroleum-contaminated soil. The influencing factors were determined by variance analysis. This proves that the interaction between key factors in the bioremediation process can be modeled, optimized, and studied by Box–Behnken design using RSM technology, which can maximize the biodegradation capacity of PAHs in soil and achieve the maximum degradation efficiency [51]. Rostampour and others used response surface methodology to study and optimize important parameters such as ethanol ratio, salt content, extraction volume, and dispersant solvent in the extraction process. Microwave-assisted extraction (MAE) technology was used in the pretreatment stage to improve the release of solid samples in aqueous solution and shorten the extraction time [52]. Marta et al. analyzed 14 PAHs in grilled and smoked muscle foods using acetonitrile as an extraction agent using response surface methodology. Matrix matching calibration curves were developed and weighted least square calibration was used to determine the optimal dosage of magnesium sulfate and sodium chloride to facilitate liquid phase separation of PAH-containing acetonitrile extraction. The results showed that the recovery rate was high and the repeatability and reproducibility met the relevant standards. Compared with the traditional method, the experimental extraction is simple and does not require adsorbents or special equipment [53]. Mohammadi et al. separated and determined PAHs in edible oil, and microwave technology was used to complete the rapid release of PAHs in the sample. Response surface methodology based on central composite design was used to study the influencing factors of the extraction process. This method is an accurate, rapid, and reliable sample pretreatment method for the extraction and determination of PAHs from different edible oil samples [54]. Dalvand et al. prepared silica/polyaniline nanofiber adsorbent to prevent the aggregation of polyaniline in the process of polymerization by combining in situ polymerization and electrospinning. The prepared NTD and gas chromatography-flame ionization detector were combined with response surface methodology to simultaneously analyze PAHs and benzene series in soil. The effective experimental variables were evaluated by introducing the RSM method designed by Box–Behnken, and the influencing experimental variables were optimized. Under the optimized conditions, a lower detection limit, a wider detection limit, an acceptable recovery rate, and reproducibility were obtained [55]. Yang et al. used 1,3,5-tris (4-aminophenyl) benzene and triformyl chloride (TAPBTMC-COF) for amide coupling reaction at room temperature, combined with solid-phase microextraction technology and response surface methodology to determine the influence of parameters on SPME efficiency. The results show that the method has a high recovery rate and can be used for the determination of PAHs in actual water samples [56]. In the experiment of simultaneous determination of 16 PAHs in barbecue samples, Kamankesh et al. used response surface methodology to optimize the factors related to microextraction efficiency. Compared with other methods, this method is simple and feasible, with short total analysis time, low solvent consumption, high recovery rate, high enrichment coefficient, good repeatability, good precision, and high feasibility [57]. Hosseini and others established a gas chromatography-flame ionization detector (GC-FID), floatation-assisted liquid-liquid microextraction (HLLME-FA) method for the determination of PAHs in water samples and designed a special extraction pool for the first time to facilitate the extraction and collection of four PAHs in water samples with low-density solvents. The data were analyzed by a regression program based on the FCCD response surface method (RSM). The optimal conditions of each variable and the effects of different factors on the extraction efficiency were studied, and the method obtained satisfactory results [58]. Mohammadi and others measured the content of 16 polycyclic aromatic hydrocarbons (PAHs) in 80 samples of 4 traditional smoked fish and found that there was a significant interaction between the volume of hydrolysate and the amount of ethanol ratio extractant and dispersant. In this study, RSM was used to describe the complete effect of each parameter in the process and evaluate the influence of the interaction between the selected variables on the extraction conditions, which can effectively extract and measure the residual PAHs in smoked fish [59]. Christopoulou and others established a matrix solid-phase dispersion extraction (MSPD) method for the determination of 16 preferred PAHs in indoor dust samples from the Environmental Protection Agency (EPA). In this study, response surface methodology based on experimental statistical design is applied. Satisfactory results are obtained in linear accuracy range and precision of the optimized experimental method. All the target analytes have high recoveries and are suitable for the analysis of PAHs in specific matrix [60]. In the determination of PAHs in smoked rice samples, Fazeli et al. designed experiments using the CCD method and investigated the effects of extraction solvent volume factor, purification cylinder type, purification solvent type, and volume on the reaction rate (BAP recovery rate). ANOVA was used to analyze the variance of 72 test data. RSM describes the full effect of each parameter in the process and includes the interaction between the variables. The BAP index of Hashmi and local Domesia smoked rice samples was determined by the optimized selection method. The BAP index of most smoked rice samples was lower than the maximum allowed level in the European Union [61]. Mollahosseini and others used mechanical stirring bar adsorption extraction MSBSE-PAN combined with GC/FID to extract and determine some low-molecular weight polycyclic aromatic hydrocarbons (PAHs) in water samples. The response surface methodology (RSM) based on central composite design (CCD) was used to optimize the adsorption time, desorption time, sample volume, and stirring speed. Under the optimum conditions, the limits of detection (LOD) and limits of eligibility (LOQ) were in reasonable range, respectively. The relative standard deviations (RSDs) of the analytes including acenaphthene (ACE), anthracene (Ant), naphthene (NAP), and phenanthrene (PHE) were less than 12.7%, and the relative recovery (RRS) was at a high level. The application of the coating saves cost and time, and the method of extracting PAHs from water samples is economical and time saving. The results show that this method is a time efficient, economic, and effective method to obtain the best extraction conditions [62].

4.2. Artificial Neural Network. The artificial neural network (ANN) is a kind of flexible mathematical structure. It can extract the basic interaction between dependent variables and independent variables with high precision by simulating the human brain's organizational structure and thinking mode. It endows computer programs with self-learning ability and can be used as a method to predict the optimization of the microchemical research process. The artificial neural network can be used as a method to predict the optimization of the microchemical research process because of its unique characteristics of nonlinearity, self-adaptation, generalization, and model independence, and some satisfactory results have been obtained in some studies.

The BP neural network is a kind of the neural network which adopts the error backpropagation training algorithm. It is a one-way propagating multilayer feedforward network composed of input layer, hidden layer, and output layer. The BP neural network adopts the supervised learning method. The process of learning algorithm is divided into two stages: the first stage is the forward propagation process, in which the actual output value of nodes at each layer is calculated from the input layer through the hidden layer, layer by layer, and nodes at each layer only accept the input of the previous node. It only affects the state of the next node. The second stage is the backpropagation process. If the output layer fails to obtain the desired output value, the error between the actual and expected output is recursively calculated layer by layer, and the error signal tends to be minimized according to this error.

The backpropagation artificial neural network model is considered as a potential application for predicting PAH concentrations in soils, and its application can help reduce the frequency of chemical analysis for on-site remediation monitoring purposes and support the decision of the end point of remediation. Huanyu et al. studied the influence of corn stalks on PAHs diffusion in soil and its related mechanism, modeled the relationship between soil properties and PAHs concentration in soil by using the backpropagation artificial neural network, and determined the predictive ability of the artificial neural network model on PAHs concentration in soil after straw returned to field. The performance of the neural network models was quantified by root mean square error (RMSE):

$$\mathrm{RMSE} = \sqrt[2]{\frac{\sum_{i=1}^{n}\left(x_i - y_i\right)^2}{n}}. \tag{2}$$

It was found that the addition of 6% corn straw amount could significantly increase the dissipation of PAHs in soil, and the addition of corn straw increased the solubility and migration of PAHs, thus improving the biodegradation of PAHs in soil. This provides a feasible option for remediation of PAHs contaminated soil [63].

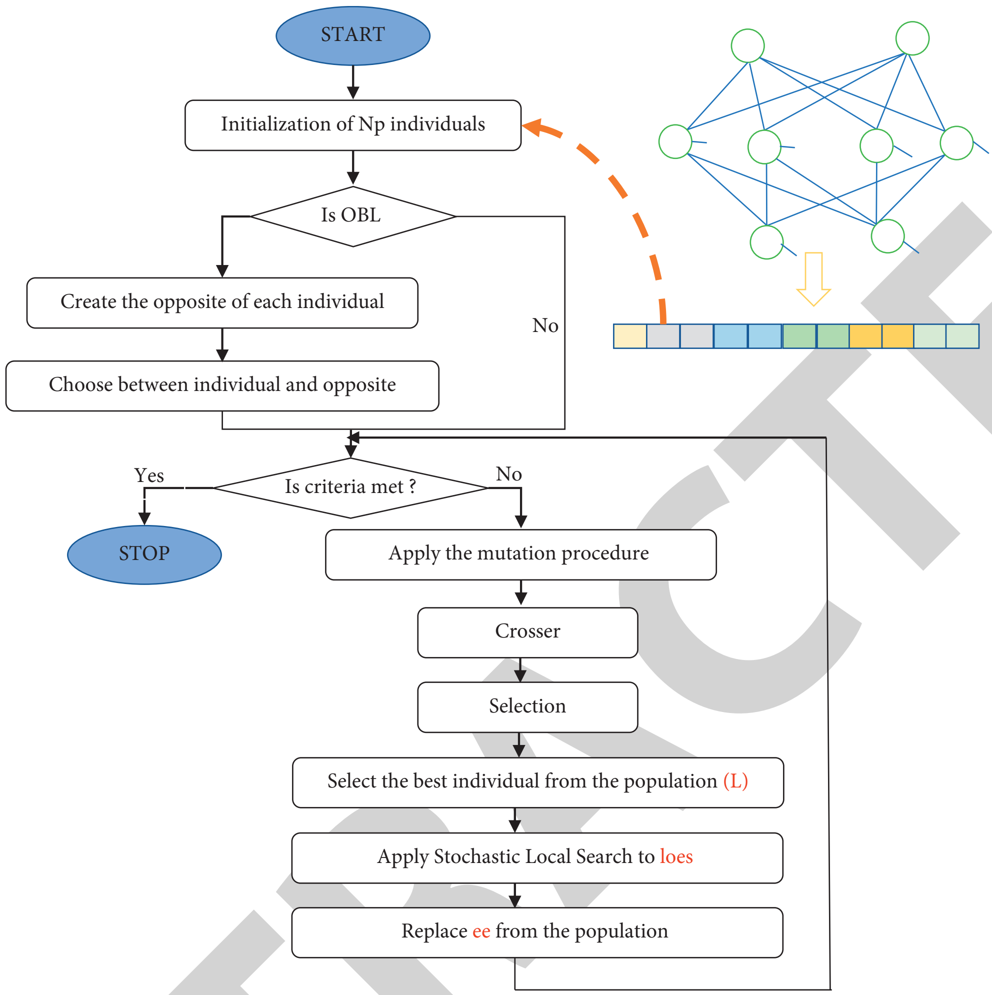

Figure 2: Scheme of the DE algorithm used to evolve the ANN parameters.

Chen et al. used the backpropagation artificial neural network to predict the content of benzo [a] pyrene in smoked sausage. The effects of smoking temperature, smoking time, and fat/lean meat ratio on BAP content were analyzed, and the nonlinear regression model and BP-ANN model were established, respectively. The BP-ANN can better explain the uncertainty and nonlinear relationship of BAP content in sausage under different smoking conditions, which further shows that the ANN model is an ideal model for predicting BAP content [64]. Xu et al. established the parameter-biodegradation relationship model of polycyclic aromatic hydrocarbons hypoxic Andrews model using the BP-ANN method, and the results showed that the back-propagation artificial neural network had high prediction accuracy and ability [65].

As one of the optimization algorithms, the differential evolution algorithm is getting more and more attention. Using Visual Studioc\Network Framework 4.0, Pirsaheb et al. modeled the formation of PAHs in meat products using artificial neural networks (ANNs) optimized by the differential evolution algorithm. The type of meat (the animal that provides the meat), the meat cut (the specific part of the animal that cuts the meat), the presence of skin, the barbecue temperature, and the time were taken as input parameters, and the output was the total PAHs value. In addition, in order to improve the quality of the initial solution, the author adopts objection-based learning (OBL), and the optimal network results are in good agreement with the experimental data. Therefore, this method can replace experiments used to predict PAH levels in various meats and reduce the consumption of resources in terms of time, experienced human resources and materials. The scheme of the DE algorithm and its integration with ANNs is shown in Figure 2 [66].

Principal component analysis is often used to extract the main characteristic variables of data. Cauchi et al. used the artificial neural network (ANN) method to qualitatively and quantitatively determine some key pollutants in drinking water at the same time and successfully determined the contents of cadmium, lead, copper, and polycyclic aromatic hydrocarbons (PAHs) such as anthracene, phenanthrene, and naphthalene in special water samples. Principal component analysis (PCA) was used as the data preprocessing technology before ANNS modeling, and the root mean square error (RMSEP) was used to measure the difference between the predicted concentration and the actual concentration, so as to obtain the optimal ANN model. This method greatly improves the ability of accurate prediction of pollutants and can be effectively used to obtain quantitative data of pollutant concentration in drinking water [67]. Wesolowski et al. used two different types of the neural network multilayer perceptual sensor (MLP) and self-organizing map (SOM) to identify changes in urban air pollutant levels throughout the year, where MLP was used to predict which heating season a sample was collected in, and SOM was used to map all samples to identify any similarities between them [68].

In recent years, along with the vigorous development of social economy and science and technology, ocean and soil also suffered from pollution in different degree; the existence of various pollutants (such as PAHs) poses a threat to the environment and biota. Therefore, how to promote the effective degradation of PAHs to design the bioremediation strategy has become one of the focuses of attention in recent years. Jing et al. established an artificial neural network model to predict the removal effect of polycyclic aromatic hydrocarbons (PAHs) in marine oil-bearing wastewater by ultraviolet radiation. Naphthalene was selected as the representative of polycyclic aromatics; 12 neurons in the hidden layer and Levenberg–Marquardt backpropagation algorithm were used to find that the number of neurons in the hidden layer would significantly affect the convergence and prediction accuracy of the network (Figure 3). The removal rate was taken as the model output. The injection rate, salinity, temperature, initial concentration, and reaction time were simulated as functions of five independent input variables. It is concluded that the neural network model can effectively predict the degradation behavior of PAHs induced by light, and the removal rate of the established neural network model is close to the measured value validation and test subset, which can accurately simulate the naphthalene removal process and reproduce the experimental results (Figure 4). The experiment operation time and material cost are saved, and the mechanism of photodegradation of PAHs is further understood, which provides a scientific basis for Marine and offshore oil and gas industry to develop corresponding treatment technology [69].

In recent years, central composite design based on the response surface methodology and artificial neural network combined with the genetic algorithm model have been used more and more in the detection of PAHs. Sachaniya et al. compared the biodegradation levels of PAHs by the response surface method and artificial neural network. The results showed that the degradation rate of PAHs predicted by the neural network model based on the mean absolute deviation and other error functions was higher than that of RSM, and the error function values of the ANN were lower. Therefore, the artificial neural network is proved to be a more reliable bioengineering tool with the best structure [70]. Mohammadi et al. used the response surface method (RSM) and artificial neural network (ANN) combined with the genetic algorithm (GA) to model and optimize the removal of pyrene from sorghum contaminated soil. In the experiment, the LM algorithm was chosen as the best training algorithm to determine the best and worst conditions for removing

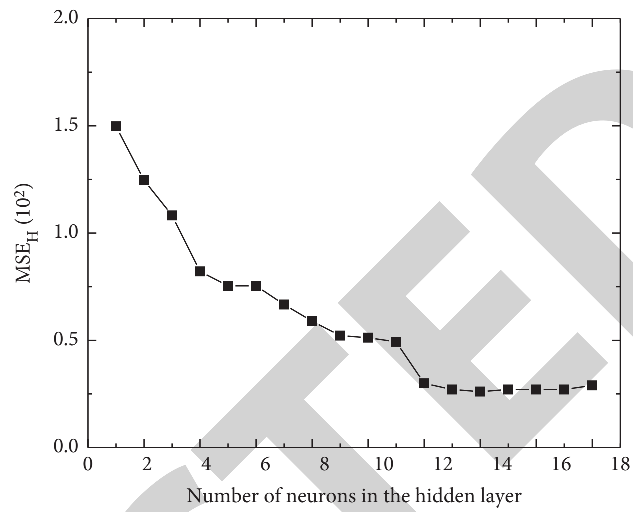

Figure 3: Relationship between the number of hidden neurons and MSE.

pyrene. The results showed that using indoleacetic acid and *Pseudomonas* could improve the removal efficiency of pyrene in soil of sorghum plants, and the prediction ability of the neural network model was obviously better than that of the RSM model [71]. Subashchandrabose et al. established the artificial neural network (ANN) and genetic algorithm (GA) models to analyze the toxicological interactions of phenanthrene and benzo [a] pyrene, as well as two kinds of heavy metals (HMS) on *Chlorella* MM3 oxidative stress. The validation of experimental data and biochemical prediction results showed that the model established by the combination of the neural network and genetic algorithm could effectively predict the toxicity of PAHs and HMS mixture to microalgae, and the relative error was only 10%. This study provides biochemically based mechanical toxicity information of microalgae exposed to mixtures of organic and inorganic pollutants, thus laying a foundation for future studies on the mechanism of microalgae mixed toxicity and the development of a better toxicity prediction model for polycyclic aromatic hydrocarbons and HMS mixtures [72].

5. Summary and Prospect

After reading a lot of literature, it is found that the pollution of polycyclic aromatic hydrocarbons (PAHs), which is one of the pollutants under optimal control in the EU, should not be underestimated. This article first introduces the characteristics and sources of polycyclic aromatic hydrocarbons and summarizes the four main sources: high temperature fume bake food contamination, food packaging contact material pollution, air pollution, and water pollution on the testing and analysis of polycyclic aromatic hydrocarbon compounds extracted or separation of the literature, through the search of pollutant source and select reasonable method for effective control of them.

In this increasingly "intelligent" era, various technologies emerge at the historic moment, which not only improve our thinking mode and methods but also make our

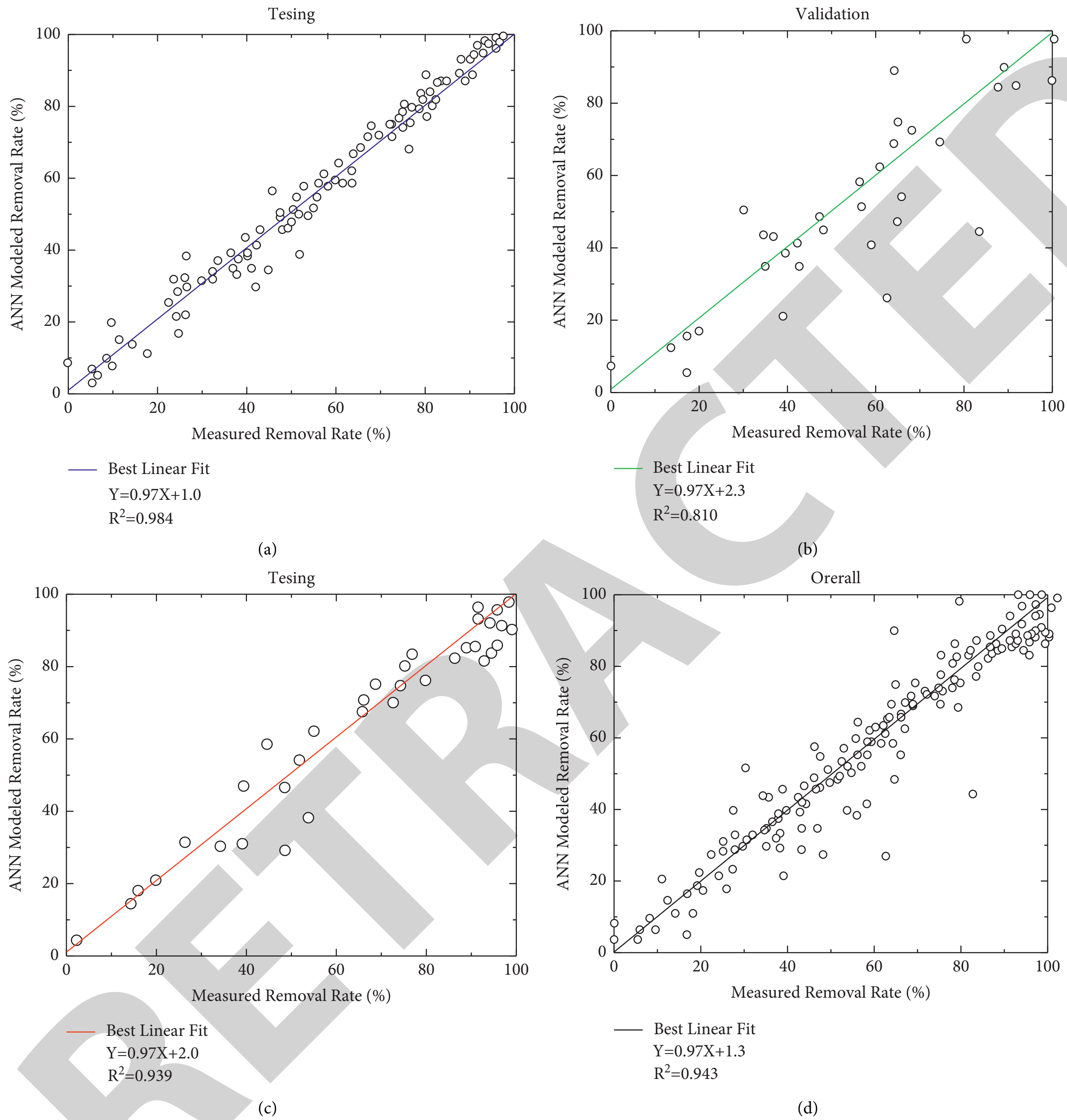

Figure 4: Comparison between ANN modeled and experimentally measured values of naphthalene removal rate for the (a) training, (b) validation, (c) testing, and (d) overall data.

experimental work more convenient. In the tens of thousands of experimental data, combined with hundreds of thousands of years ago, the computer has shown unparalleled advantages. The numerical simulation method and response surface can be used to process the data in batches and select the optimal solution among the numerous data. The emergence of the artificial neural network makes the computer have the ability of self-learning, simplifies the complex experimental operation, and saves time. It has strong learning ability and fault tolerance and can adapt to various evaluation environments. The prediction can be made through the establishment of the model, so as to provide a way and help for the targeted pollution prevention and control in advance.

In a word, with the development of computing hardware and theoretical methods, big data, deep learning, and artificial intelligence will continue to play an increasingly important role in the field of chemistry and chemical engineering and will develop towards a more intelligent and efficient direction.

Data Availability

The data used to support the findings of this study are available from the corresponding author upon request.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

Acknowledgments

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