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Interfacial Mechanisms, Influencing Factors and Research Progress of Nanocomposite Membranes for Synergistic Removal of PFAS and Antibiotics in Water

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Abstract. Per and polyfluoroalkyl substances (PFAS) and antibiotics are two typical emerging water contaminants, and conventional water treatment processes hardly achieve their simultaneous deep removal. Nanocomposite membranes couple polymer-based size-exclusion filtration with interfacial adsorption of nanofillers, which can treat PFAS-antibiotic co-contaminated water synergistically and have become a research hotspot for emerging pollutant remediation. This paper illustrates the interfacial interaction mechanisms between PFAS, antibiotics and nanocomposite membranes, summarizes material features of carbon-based, MOF, two-dimensional layered and organic-modified fillers as well as regulation rules for membrane fabrication, and analyzes the adsorption-filtration synergistic removal mechanisms. The effects of membrane structure, water matrix and operating parameters on treatment performance are discussed. Current bottlenecks including insufficient direct experimental data under co-contamination conditions and unclear site competition as well as long-term stability are pointed out. Prospects are proposed for material optimization, real-water tests and practical engineering applications.

Keywords: nanocomposite membrane, per and polyfluoroalkyl substances (PFAS), antibiotics, adsorptionfiltration synergy, interfacial interaction, emerging contaminants

1. Introduction

Per- and polyfluoroalkyl substances (PFAS) are synthetic organic compounds containing at least one perfluoromethyl or perfluoromethylene structural unit, with properties such as heat resistance, chemical corrosion resistance, hydrophobicity and oleophobia, and have long been used in fire-fighting foams, textile finishing, electronics manufacturing, food packaging and surfactants. Li Jian et al. pointed out that PFAS are numerous in types and continuously detected in various environmental media, and their trace monitoring and risk identification have become an important basis for emerging pollutant control [1]. Crone et al. systematically reviewed the occurrence of PFAS in drinking water sources and the status of their treatment, and considered perfluorocarboxylic acids (PFCA) and perfluorosulfonic acids (PFSA) the most concerned categories [2]; Ateia et al. further emphasized that short-chain and ultrashort-chain PFAS have high water solubility and strong

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mobility, and conventional adsorption materials are more prone to rapid breakthrough when treating such pollutants [3].

Antibiotics mainly come from medical discharge, livestock and poultry and aquaculture, pharmaceutical wastewater and domestic sewage. Qi Yabing et al. pointed out in a review of antibiotic wastewater treatment technologies that antibiotic wastewater is characterized by complex composition, poor biodegradability and significant biological toxicity, and a single physical, chemical or biological process is often difficult to stably meet discharge standards [4]. The environmental significance of antibiotics is not limited to parent compound residues. Wu Xiaojian et al. summarized the carriage of drug-resistant bacteria and antibiotic resistance genes by biofilms on microplastic surfaces, and considered that mobile genetic elements such as plasmids, integrons and transposons increase the risk of horizontal gene transfer [5], so antibiotic pollution control should take into account both the reduction of chemical residues and the blocking of resistance spread risk.

Conventional treatment processes are difficult to simultaneously meet the requirements of deep removal of low-concentration emerging pollutants, continuous operation and final disposal. Zhang Yanhong et al. compared nanofiltration, reverse osmosis, forward osmosis and various modified membranes and pointed out that although membrane technology has advantages such as compact devices and stable operation, its rejection is jointly affected by membrane structure, pollutant properties and water quality conditions [6]. For PFAS, Das and Ronen considered that ordinary low-pressure membranes are difficult to stably remove dissolved components with smaller molecular scales, while dense nanofiltration or reverse osmosis faces concentrate treatment and higher pressure requirements [7]. Gagliano et al. further pointed out that the performance of adsorption materials such as activated carbon is obviously affected by PFAS chain length, natural organic matter competition and regeneration methods, and short-chain PFAS are especially prone to early breakthrough [8]. In this regard, the core idea of nanocomposite membranes is to fix nanomaterials with specific pores, functional groups and surface charges in a continuous membrane structure, so that the membrane is both a hydraulic sieving medium and a controllable interfacial adsorption reactor. Geng Qiwei et al. summarized the preparation of MOF-polymer composites as routes such as direct blending, in-situ synthesis in the polymer matrix and in-situ growth on the polymer surface, showing that the membrane structure can simultaneously undertake filler fixing and mass transfer regulation functions [9]. Lu Hao et al. pointed out that MOF porous materials can achieve adsorption, catalysis and multi-mechanism interfacial interactions through tunable pore size, unsaturated metal sites and organic ligands [10]. This paper will systematically expound the basic principles of nanocomposite membranes for the removal of PFAS and antibiotics and their advantages and limitations in practical application, from the aspects of pollutant structural characteristics, pollutant-membrane material interactions, membrane material systems, synergistic removal mechanisms, influencing factors, and existing problems and development trends.

2. Interfacial mechanisms between PFAS, antibiotics and nanocomposite membranes

2.1. Structural characteristics of PFAS molecules and interfacial interaction mechanisms

PFAS usually consist of charged or ionizable hydrophilic head groups and perfluorinated or polyfluorinated carbon chains, with a typical amphiphilic structure. Most perfluorocarboxylic acids and perfluorosulfonic acids exist as anions at common environmental pH, so the fixed charge on the membrane surface first determines whether they are repelled or attracted at the interface. When Fujioka et al. studied the nanofiltration behavior of PFAS with different functional groups, they found that molecular size, functional group type and local negative charge jointly affect rejection.

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For a negatively charged selective layer, Donnan exclusion can reduce the probability of anionic PFAS entering the pores, while positively charged sites such as protonated amine groups and quaternary ammonium groups can achieve interfacial enrichment through electrostatic attraction or anion exchange [11].

Electrostatic interaction is especially important for short-chain PFAS. He Kunzhen et al. introduced polyethyleneimine (PEI) PEI into PAN nanofiber membranes and found that with the increase of amine sites, the PFOA adsorption capacity improved significantly; the Langmuir saturated adsorption capacity of the 3% PEI sample reached 1145.55 mg/g, and the adsorption was stronger under acidic conditions, indicating that the electrostatic binding between protonated amine groups and PFOA anionic head groups is the main driving force. The study also showed that the functional polymer needs to be distributed on the fiber surface or pore walls in a form accessible to water flow before the number of functional groups can be converted into effective adsorption sites [12].

Hydrophobic interaction is mainly reflected in the partitioning of PFAS fluorocarbon chains from the aqueous phase into nonpolar domains. After synthesizing multiple types of adsorption materials, Gagliano et al. pointed out that long-chain PFAS usually have a stronger adsorption tendency than short-chain PFAS, because the increase of chain length enhances the hydrophobic driving force and interfacial activity. One thing to note is that although overall excessive hydrophobicity of the material may enhance the enrichment of long-chain PFAS, it will reduce water wettability and aggravate natural organic matter fouling [8]. Therefore, a more reasonable design is to form an amphiphilic structure in which a hydrophilic water-transport skeleton and local hydrophobic microdomains coexist, rather than simply increasing the hydrophobicity of the membrane.

The carboxylate or sulfonate groups of PFAS can also form hydrogen bonds, ionic bridging and coordination with hydroxyl, amine, metal oxide or MOF metal nodes on the membrane surface. Lu Hao et al.'s summary of MOF removal of organic pollutants from water showed that unsaturated metal sites, pore confinement and organic ligands can jointly improve interfacial binding, but water molecules, inorganic anions and natural organic matter also compete for active sites [10].

Chain length, head group type, branching structure and hydrated size jointly determine the adsorption and sieving behavior of PFAS. The ZIF-L/PEI thin-film nanocomposite membrane prepared by Bi et al. showed an overall upward trend in the rejection of PFHxA, PFHxS, PFOA and PFOS with increasing chain length, indicating that size, interfacial affinity and charge effects are coupled with each other [13]. Zhi et al. improved the rejection of short-chain PFAS by tuning the surface charge of the nanofiltration membrane, showing that the removal of short-chain components cannot rely only on reducing the pore size, and the fixed charge density in the pores should also be increased [14]; the results of Fujioka et al. on functional groups and local charges also support this judgment [11].

2.2. Structural characteristics of antibiotic molecules and interfacial interaction mechanisms

Antibiotics are of many types and complex functional groups; the common tetracyclines, quinolones, sulfonamides, macrolides, β-lactams and aminoglycosides contain aromatic rings, heterocycles, carboxyl, hydroxyl, amino and amide groups respectively. Most antibiotics have multi-step acid-base dissociation and may exist as cations, zwitterions, anions or neutral species at different pH. Wang Yujia et al. pointed out that the adsorption and catalytic performance of MOF in removing antibiotics is obviously affected by antibiotic structure, pH, material active sites and water quality conditions [15]. In addition, because different antibiotics carry different charges at different pH, electrostatic attraction or repulsion may occur between them and the membrane surface.

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Therefore, the rejection of antibiotics by the membrane cannot be judged only by molecular weight; the charged state of the antibiotics and the electrical property of the membrane surface should also be considered.

Carbon materials with aromatic conjugated structures, PDA and MOF organic ligands can undergo π-π stacking with tetracycline, quinolone and some sulfonamide antibiotics. Zhao Fengmin et al. considered that the adsorption performance of activated carbon for antibiotics depends on pore structure and surface chemical properties, and oxygen-containing and nitrogen-containing functional groups change hydrogen bonding, electrostatic and aromatic interactions [16]. The Fe3O4-reduced graphene oxide composite prepared by Wang Xiaofeng et al. showed higher adsorption capacity for tetracycline antibiotics than single Fe3O4, confirming the complementary synergistic effect between the carbon-based aromatic interface and metal oxide active sites [17].

Hydrogen bonds come from the donor-acceptor matching between the hydroxyl, carbonyl, amino and amide groups of antibiotics and groups such as -OH, -NH2 and -COOH in membrane materials. The MOF-801@PDA@PAN nanofiber membrane constructed by Nian Qixun can simultaneously adsorb 32 antibiotics of six major classes within a relatively short time, and the mechanism analysis showed that electrostatic interaction, hydrogen bonding, π-π interaction and metal complexation all participate [18]. The study also suggested that liquid-film mass transfer, diffusion inside the membrane and site binding all affect the adsorption rate, proving that sufficient active sites combined with an open structure accessible to water flow can be converted into practically usable pollutant removal capacity.

Metal coordination plays a particularly key removal role for tetracycline and quinolone antibiotics containing adjacent hydroxyl, carbonyl or carboxyl groups. Wang Xiaofeng et al. found that the adsorption capacities of Fe3O4@rGO for different tetracycline antibiotics differ, reflecting the different binding strengths of molecular structures with metal oxides and carbon-based surfaces [17]. After introducing HKUST-1 into a polysulfone membrane, Cevallos-Mendoza et al. obtained high removal rates for oxytetracycline, tetracycline and chlortetracycline, and regarded the complexation of Cu nodes with tetracycline as one of the key interactions [19]. Wang Yujia et al. also pointed out that although metal nodes can improve antibiotic affinity, their stability, ion leaching and competing ligand effects must be included in material evaluation [15].

Compared with PFAS, the interfacial interaction of antibiotics has stronger molecular specificity. Highly polar aminoglycosides have few aromatic structures and rely more on hydrogen bonding and electrostatic interaction; tetracyclines and quinolones can undergo both π-π interaction and metal coordination; macrolides have larger molecular sizes, and steric hindrance and pore sieving contribute more prominently. Therefore, functional membranes for water bodies with multiple coexisting antibiotics should avoid various pollutants competing for the same type of sites through the spatial partitioning of aromatic sites, polar sites and stable metal nodes.

2.3. Limitations of single adsorption and single membrane filtration removal mechanisms

Single adsorption can remove pollutants that are small in size and difficult to be directly retained by membrane pores, but it is limited by the limited number of active sites on the adsorption material. As time goes on, the adsorption sites will gradually saturate, and pollutants may desorb or break through. Natural organic matter also competes with PFAS for adsorption sites, and the interaction between short-chain PFAS and materials is weaker, so breakthrough is more likely to occur. The adsorption effect of antibiotics is also affected by material pore structure, surface functional groups, solution pH and coexisting substances. For MOF materials, inorganic ions and organic matter in water may also occupy part of the active sites, leading to the decay of adsorption capacity.

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Powdered adsorbents have problems of difficult solid-liquid separation and particle loss. When the adsorbent is regenerated, salts, acids and bases or organic solvents are usually needed, and these processes will produce regeneration waste liquid containing high concentrations of pollutants. Fixed beds are convenient for continuous treatment, but long-term operation may have problems such as bed clogging, pressure rise and reduced mass transfer speed. Therefore, although single adsorption can reduce the concentration of pollutants in water, it still has shortcomings such as easy saturation, difficult recovery and secondary treatment of regeneration waste liquid.

Single membrane filtration has advantages such as small equipment footprint and continuous water production, but its removal effect largely depends on membrane pore size, membrane surface charge and operating pressure. Ordinary microfiltration and ultrafiltration membranes have large pore sizes and can hardly stably remove dissolved antibiotics by size sieving alone; although nanofiltration and reverse osmosis membranes can improve the rejection rate, they are also prone to problems such as membrane fouling, high energy consumption and difficult treatment of concentrate. For PFAS, membrane separation mainly retains pollutants and concentrates them into the concentrate, and does not really destroy the molecular structure of PFAS, so it needs to be used in combination with subsequent degradation or harmless treatment technologies.

In addition, the membrane material itself may temporarily adsorb pollutants, creating an adsorption illusion of high rejection. As the adsorption sites on the membrane surface and in the pores are gradually occupied, pollutants will begin to pass through the membrane and the effluent concentration will rise. Therefore, evaluating membrane treatment effect cannot rely only on the instantaneous removal rate; the pollutant breakthrough curve, the treated water volume per unit membrane area, the stable flux, the pollutant residue in the membrane and the performance after membrane regeneration should also be examined. Only when good removal effect and water flux can be maintained after a long period of operation can it be shown that the membrane has a relatively stable treatment capacity.

3. Nanocomposite membrane material systems and functional characteristics

3.1. Classification of functional nanofillers and adsorption characteristics

3.1.1. Carbon-based nanomaterials

The mainstream types of carbon-based nanomaterials include graphene oxide (GO), reduced graphene oxide, carbon nanotubes, activated carbon nanoparticles and carbon nanofibers. Zhao Fengmin et al. pointed out that the pore structure of carbon materials determines the space that pollutants can enter, while the aromatic conjugated structure and surface oxygen-containing and nitrogen-containing groups provide π-π stacking, hydrophobic interaction, hydrogen bonding and charge regulation respectively. For PFAS, nonpolar carbon domains are more conducive to the partitioning of long-chain components; for antibiotics, aromatic surfaces are especially suitable for the enrichment of tetracycline, quinolone and sulfonamide molecules [16].

Compositing carbon-based materials with metal oxides or functional polymers can introduce new coordination and charge sites while maintaining a large specific surface area. Wang Xiaofeng et al. found that after Fe3O4 nanoparticles were uniformly loaded on rGO, the adsorption of chlortetracycline, tetracycline and oxytetracycline was better than that of a single component, reflecting the complementary role of the carbon-based interface and metal sites. Fixing such materials further into membranes can reduce the difficulty of powder recovery and shorten the mass

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transfer distance, but lamellar stacking, particle agglomeration, interfacial voids and potential filler shedding must also be controlled [17].

3.1.2. MOF-series functional fillers

Metal-organic frameworks (MOF) are composed of metal nodes and organic ligands, with regular channels, tunable pore size, high specific surface area and rich coordination sites, and are one of the most representative functional fillers in nanocomposite membranes. Lu Hao et al. pointed out that MOF can remove organic pollutants from water through pore sieving, electrostatic interaction, hydrogen bonding, π-π interaction and metal coordination [10]. Wang Yujia et al. summarized that Fe-MOF can both adsorb antibiotics and promote antibiotic degradation under light conditions [15]. Geng Qiwei et al. pointed out that combining MOF with polymer membranes can fix the originally dispersed powder materials on the membrane surface or membrane fibers, thereby reducing material loss and making recovery and reuse more convenient [9].

Bi et al. prepared a ZIF-L/PEI thin-film nanocomposite membrane, which maintains a high water flux while achieving good rejection of both long-chain and short-chain PFAS. This shows that MOF channels, PEI surface charge and the sieving effect of the nanofiltration membrane can jointly improve the removal of PFAS. The HKUST-1@polysulfone membrane prepared by Cevallos-Mendoza et al. also showed that the metal sites and channel structure in MOF can improve the membrane's ability to remove tetracycline antibiotics.

Therefore, the role of MOF is not just to provide a larger adsorption area; more importantly, it can simultaneously adjust the pore structure, surface charge and adsorption sites of the membrane, allowing the sieving filtration of the membrane matrix and the interfacial adsorption of fillers to work at the same time, improving the overall removal of pollutants from water.

3.1.3. Two-dimensional layered materials

Two-dimensional layered materials include GO, transition metal carbides or nitrides (MXene), layered double hydroxides, two-dimensional MOF and two-dimensional covalent organic frameworks (COF). The interlayer channels formed by nanosheet stacking have a spatial confinement effect, which can achieve size sieving by adjusting the interlayer spacing, and generate Donnan exclusion by using the surface charge of the sheets. The anionic covalent organic framework membrane prepared by Nguyen et al. used regular channels and a negatively charged surface to improve the rejection of PFAS while reducing the rejection of inorganic salts.

Two-dimensional materials can also undertake conductive and self-cleaning functions. The Cu-HHTP/PVDF conductive membrane constructed by Hu et al. can mitigate fouling electrochemically while maintaining high antibiotic rejection, which shows that two-dimensional materials can remove pollutants through pore sieving and surface adsorption, and can also use conductivity to improve the long-term operation of the membrane. However, two-dimensional materials also have problems such as decreased water flux caused by sheet stacking, increased interlayer spacing in water, and sheet shedding after long-term operation. In this regard, their stability can be improved by crosslinking, adding rigid support materials or strengthening the fixation on the support layer.

3.1.4. Organically modified functional fillers

Organic functional components mainly include polyethyleneimine (PEI), polydopamine (PDA), quaternized polymers, chitosan, cyclodextrin, ionic liquids and molecularly imprinted polymers. PEI

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is rich in primary, secondary and tertiary amines and can form high-density protonated sites under acidic to neutral conditions, suitable for capturing anionic PFAS; PDA has excellent adhesiveness, and its aromatic rings, catechol and amine groups can simultaneously provide π-π, hydrogen bonding and subsequent anchoring sites. He Kunzhen et al.'s research showed that polyethyleneimine can provide positively charged adsorption sites for PFOA [12]; Nian Qixun used PDA to fix MOF on the surface of PAN nanofibers, improving the stability and antibiotic adsorption capacity of the material [18]; Wan et al. prepared a dual-function PFAS adsorption membrane using quaternary ammonium groups and hydrophobic structures. Among them, the positively charged quaternary ammonium groups can attract the negatively charged head groups of PFAS, and the hydrophobic structure can interact with the fluorinated carbon chains of PFAS. The two actions jointly improved the adsorption and rejection of PFAS by the membrane [20].

Organically modified materials are easy to design chemically and usually have good compatibility with polymer membranes, but they also have some shortcomings. For example, some materials may swell in water, functional groups may be lost during long-term operation, and positively charged surfaces may also adsorb natural organic matter, aggravating membrane fouling. He Kunzhen's team experimentally confirmed that appropriately increasing the PEI doping ratio can increase PFOA adsorption sites, but when the PEI content is too high, local aggregation may occur and affect the pore structure of the membrane [12]. Therefore, the amount of organic functional materials is not the more the better; when screening the optimal doping amount, three indicators need to be considered at the same time: the adsorption capacity of the material, the integrity of the membrane pore structure, and the long-term operation stability.

Table 1. Structural characteristics, target pollutants and core actions of four mainstream nanofillers

Filler category	Typical materials	Structural advantages	Main target pollutants	Core interfacial actions	Existing defects
Carbon-based nanomaterials	rGO, carbon nanotubes	High specific surface area, aromatic skeleton	Tetracyclines, quinolones, long-chain PFAS	π-π stacking, hydrophobic partitioning	Sheets prone to stacking, pure water flux decreases
MOF fillers	ZIF-L, HKUST-1, Fe-MOF	Tunable pore size, rich metal active sites	PFAS, various antibiotics	Coordination, sieving, electrostatic adsorption	Powder easy to shed, moderate stability in aqueous environments
Two-dimensional layered materials	MXene, COF, LDH	Interlayer confinement, conductive	Short-chain PFAS, small-molecule antibiotics	Donnan exclusion, electrochemical self-cleaning	Interlayer spacing swells in water, sheet peeling
Organically modified fillers	PEI, PDA, quaternary ammonium polymers	Easy-to-regulate surface charge, good compatibility	Anionic PFAS, polar antibiotics	Electrostatic attraction, hydrogen bonding	Swelling in water, loss of functional groups

As shown in Table 1, carbon-based nanomaterials, MOF fillers, two-dimensional layered materials and organically modified fillers target the removal of antibiotics, PFAS and other pollutants through π-π stacking, coordination/sieving, Donnan exclusion and electrostatic/hydrogen bonding actions respectively, but each faces bottlenecks such as sheet stacking, poor water stability, swelling in water and loss of functional groups, which restrict their long-term application. Therefore, future work needs to focus on composite modification or structural optimization to balance interfacial activity and operational stability.

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3.2. Common preparation methods of nanocomposite membranes and structure regulation rules

Blending-phase inversion is a common preparation route for polymer nanocomposite membranes such as polysulfone, polyethersulfone, polyvinylidene fluoride (PVDF) and PAN. After nanofillers are added to the casting solution, they change the solvent-nonsolvent exchange rate, which in turn affects finger-like pores, sponge-like pores, surface pore size, porosity and hydrophilicity. Geng Qiwei et al. pointed out that the direct blending method is relatively simple in process and easy to scale up, but filler sedimentation and agglomeration lead to uneven pore structure and interfacial defects; Chen Yi'ang et al. also emphasized that powder materials such as MOF also need to consider mechanical strength and processing and forming issues in practical application.

Interfacial polymerization is suitable for constructing thin-film composite or thin-film nanocomposite nanofiltration layers. Nanofillers can be dispersed in the aqueous phase, the organic phase or on the surface of the support layer, and participate in pore size and surface charge regulation during the formation of the polyamide selective layer. The ZIF-L/PEI thin-film nanocomposite membrane prepared by Bi et al. showed that reasonably controlling the position and surface properties of the fillers can improve the membrane's rejection of PFAS while maintaining a high water flux. However, if the filler is not tightly bound to the polymer, voids may appear between the two, allowing pollutants to pass through these voids; if the filler is wrapped too thickly by the polymer, the pores will be blocked and the adsorption sites covered.

Electrospinning can prepare nanofiber membranes with high porosity, high specific surface area and low mass transfer resistance, suitable for building flow-through adsorption media. Functional components can be directly blended into the spinning solution, or fixed after fiber formation by PDA coating, layer-by-layer self-assembly, in-situ growth or chemical grafting. He Kunzhen et al. introduced PEI by blend electrospinning, and Nian Qixun used PDA as an intermediate layer to fix MOF-801. However, the pore size of ordinary nanofiber membranes is usually large, and it is difficult to stably retain small-molecule pollutants by their own pores alone, so a thinner selective layer, surface coating or multilayer membrane structure is often needed.

Vacuum filtration, pressure-assisted assembly and layer-by-layer self-assembly are often used to prepare two-dimensional sheet membranes or polyelectrolyte multilayer membranes. By adjusting the nanosheet size, the number of deposited layers, the degree of interlayer crosslinking and rigid spacers, the channel length, interlayer spacing and surface charge can be controlled. In-situ growth can anchor MOF or COF directly on the support layer, reducing particle shedding and forming continuous channels.

As shown in Figure 1, by comparing the various preparation processes, membrane structure regulation can be summarized into four core rules: the doping ratio of nanofillers has an optimal range, and both too high and too low weaken the treatment performance; the uniformity of filler dispersion in the casting solution directly determines the actual utilization rate of effective adsorption sites; the three parameters of membrane pore size, overall porosity and selective layer thickness simultaneously constrain the membrane's stable flux and molecular sieving capacity; and the interfacial compatibility between filler and polymer determines the long-term operation stability of the composite membrane and the risk of bypass pollutant permeation.

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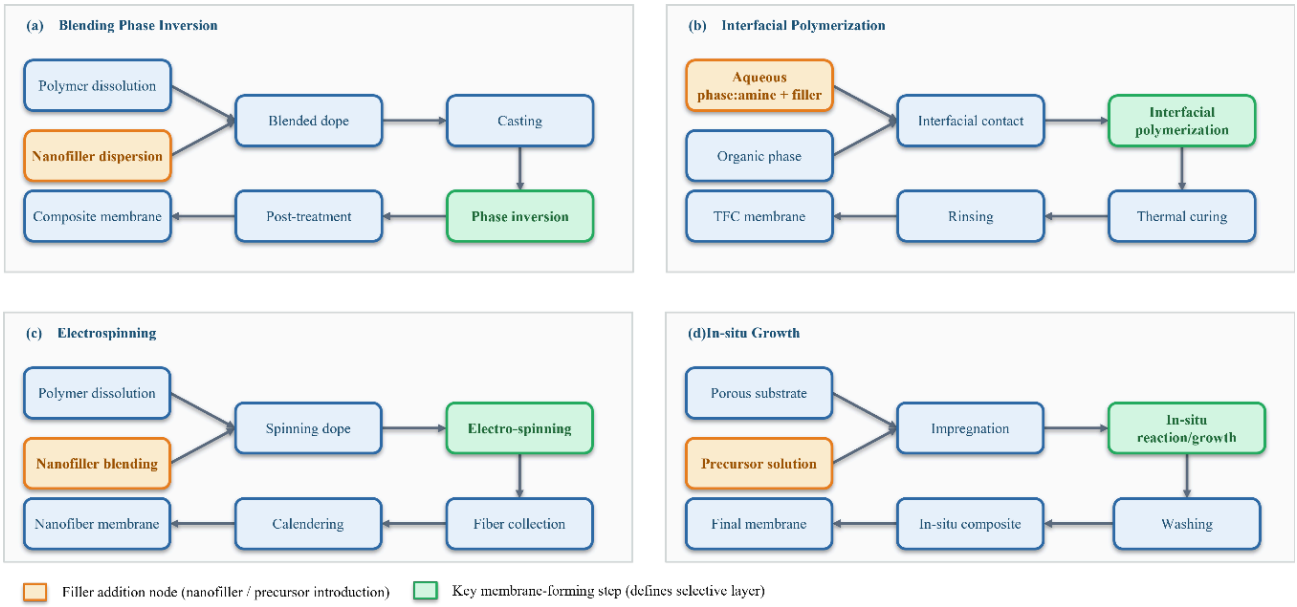


Figure 1. Schematic diagram of the four preparation processes of nanocomposite membranes

4. Core mechanisms of adsorption-filtration synergy in nanocomposite membranes

4.1. Core logic of the synergy mechanism

Adsorption-filtration synergy is not a simple addition of the adsorption rate and the rejection rate, but lets pollutants be affected by membrane pore sieving and surface adsorption at the same time as they pass through the membrane. The analyses of Geng Qiwei et al. and Lu Hao et al. showed that the filtration process can change the path and probability for pollutants to reach adsorption sites, and the adsorption process in turn reduces the effective probability of pollutants passing through the membrane pores. Therefore, the membrane does more than filter; it can also use the adsorption sites on the pore walls to improve the removal of pollutants.

The whole process can be simply understood as "sieve first, then adsorb". Molecules that are relatively large or repelled by like charges are first retained on the membrane surface; small molecules that can enter the pores continue to contact the nano sites on the pore walls and are fixed through electrostatic, hydrophobic, hydrogen bonding, π-π or coordination actions; the continuous water flow can also keep bringing new pollutants to the membrane surface and pores, so that a limited mass of filler obtains a high site utilization rate.

The goal of synergy design is not to let all substances be strongly adsorbed, but to let water pass quickly while target pollutants are slowed down and fixed. Excessive hydrophobicity increases hydraulic resistance and organic fouling, and excessive hydrophilicity may weaken the hydrophobic enrichment of long-chain PFAS; too strong site binding makes regeneration difficult, and too weak binding makes pollutants easily re-released during operation. Therefore, when designing nanocomposite membranes, the pore structure, surface charge, hydrophilicity-hydrophobicity of the membrane and the residence time of pollutants in the membrane need to be considered at the same time, so that the two actions of filtration and adsorption can interact well.

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4.2. Filtration and sieving mechanism

Membrane filtration first relies on membrane pores to sieve pollutants. Generally speaking, the larger the pollutant molecule, the less easily it passes through smaller membrane pores. When the size of a pollutant is close to the pore size, even a slight reduction of the pore or an adsorption layer formed on the membrane surface may obviously improve the rejection. In addition to molecular size, the membrane surface charge also affects whether charged pollutants can pass. Therefore, the rejection of pollutants by the membrane is usually jointly determined by the pore size and the electrical property of the membrane surface.

For PFAS, long-chain PFAS are usually more easily retained by the membrane than short-chain PFAS. On the one hand, long-chain PFAS molecules are relatively large and have more difficulty passing through smaller membrane pores; on the other hand, the interaction between long-chain PFAS and membrane materials is usually stronger. Therefore, the rejection of PFOA and PFOS is often higher than that of short-chain PFAS such as PFBA and PFHxA. The composite membrane prepared by Bi et al. also showed a trend of higher rejection of long-chain PFAS than short-chain PFAS [13]. Fujioka et al. pointed out that the functional groups and charged state of PFAS also affect membrane separation [11]; Zhi et al. improved the rejection of short-chain PFAS by enhancing the negative charge on the membrane surface [14]. This shows that for short-chain PFAS of smaller size, besides reducing the membrane pores, the charge repulsion on the membrane surface can also be used to improve removal.

The sieving of antibiotics is more affected by molecular configuration and pH. Larger molecules such as tetracyclines and macrolides are easily controlled by steric hindrance, and small-molecule sulfonamides are more likely to pass through if they also lack charge repulsion. The studies of Zhang Yanhong et al. and Nian Qixun showed that the membrane separation of antibiotics is related to molecular size, and is also affected by pH, the charged state of the antibiotics, membrane surface properties and other substances in the water [6, 18].

4.3. Nano-interfacial adsorption mechanism

Nano-interfacial adsorption reduces the probability of pollutants migrating to the permeate side by increasing their residence time and binding energy in the membrane. For PFAS, protonated amine groups or quaternary ammonium groups are responsible for attracting anionic head groups, and hydrophobic cavities and carbon-based surfaces are responsible for accommodating fluorocarbon chains. The studies of He Kunzhen et al. and Wan et al. showed that when the membrane material has both positively charged adsorption sites and hydrophobic structures, PFAS can be adsorbed from two aspects [12, 20]. Combining these adsorption actions with membrane pore sieving can further improve the removal of long-chain and short-chain PFAS.

The structure of antibiotics is more complex than that of PFAS, so multiple adsorption actions usually need to participate together. In the Fe3O4@rGO composite prepared by Wang Xiaofeng et al., the graphene surface can interact with the aromatic structures of antibiotics, and Fe3O4 can also provide additional adsorption sites [17]. The MOF-801@PDA@PAN membrane prepared by Nian Qixun can adsorb antibiotics through π-π interaction, hydrogen bonding, electrostatic interaction and metal coordination [18]. In the HKUST-1@polysulfone membrane prepared by Cevallos-Mendoza et al., the Cu metal nodes can coordinate with tetracycline antibiotics [19]. From these studies it can be seen that when treating multiple antibiotics, membrane materials with different types of adsorption sites are usually better able to adapt to pollutants of different structures.

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One thing to note is that the number of sites is not equal to the number of effective sites. If nanoparticles are completely embedded in the polymer, the theoretical specific surface area cannot be converted into a water-accessible area. If fillers are concentrated on the membrane surface, they may cause clogging, increased roughness and particle shedding. Geng Qiwei et al. pointed out that different composite methods affect the position of functional materials in the membrane and whether pollutants can reach these materials [9]; Chen Yi'ang et al. pointed out that the water stability, mechanical strength and processability of materials also affect their long-term use effect [21]. Therefore, when preparing nanocomposite membranes, functional materials should be distributed as much as possible in positions that the water flow can reach, while ensuring that these materials are firmly fixed in the membrane.

4.4. Adsorption-filtration synergistic enhancement mechanism

Nanocomposite membranes fix materials with different adsorption functions on the membrane surface or in the membrane pores, so that PFAS and antibiotics are subjected to filtration and adsorption at the same time during the filtration process. Filtration can first restrict part of the pollutants from passing through the membrane, and the PFAS and antibiotics that can enter the membrane pores will continue to contact the adsorption sites in the membrane. Therefore, filtration provides continuous water flow and contact conditions for adsorption, and adsorption further removes small-molecule pollutants that are difficult to retain by filtration alone.

Because the structures of PFAS and antibiotics are different, different types of adsorption sites can be set in the same membrane. For PFAS, positively charged groups can adsorb their negatively charged head groups, and hydrophobic structures can further interact with the fluorinated carbon chains. For antibiotics, aromatic structures, oxygen-containing or nitrogen-containing functional groups and metal sites can be used for adsorption through π-π interaction, hydrogen bonding, electrostatic interaction and metal coordination.

Therefore, after PFAS and antibiotics enter the same nanocomposite membrane, they do not go through two completely independent treatment processes, but are subjected to filtration and adsorption at the same time in the same filtration process. In terms of filtration, the membrane pores can restrict their passage according to the molecular size of the pollutants, and the membrane surface charge will also attract or repel charged PFAS and antibiotics, so that part of the pollutants is retained; pollutants that can continue to enter the membrane pores further contact the adsorption sites in the membrane. In this way, filtration reduces the chance of PFAS and antibiotics passing through the membrane and gives the pollutants that enter the pores more opportunities to contact adsorption sites, and adsorption further fixes the pollutants that filtration can hardly completely retain, so that filtration and adsorption cooperate in the same membrane and jointly improve the removal of the two types of pollutants.

5. Key influencing factors of the adsorption-filtration synergistic effect

5.1. Influence of intrinsic membrane structure parameters

The amount of filler added affects the adsorption sites and water flow channels in the membrane. When the filler is too little, the adsorption sites that can be provided are limited; adding an appropriate amount of filler can improve the hydrophilicity, porosity and number of adsorption sites of the membrane. However, when too much filler is added, particles easily aggregate, which may clog the membrane pores and may also form voids between the filler and the polymer, making the

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water flux and pollutant rejection unstable. Therefore, more filler is not necessarily better; its dispersion and its actual role in the membrane also need to be considered at the same time.

The three parameters of average membrane pore size, overall porosity and selective layer thickness simultaneously constrain the two actions of filtration and adsorption. When the membrane pores are small, it is favorable for filtering larger pollutants, but the resistance for water to pass through the membrane also increases; when the membrane pores are large, water passes more easily, but some small-molecule PFAS and antibiotics also pass through the membrane more easily. Therefore, pores of different sizes can be used in combination, so that the larger pores ensure water passage, the smaller pores are responsible for filtration, and adsorption sites are set on the pore walls, so that small-molecule pollutants entering the pores are further adsorbed.

The uniformity of the distribution of fillers inside the membrane matrix is also a key parameter. If fillers such as MOF and carbon materials are completely wrapped by the polymer, pollutants in the water can hardly reach the adsorption sites inside them. If a large number of particles are concentrated on the membrane surface, they may cause membrane pore clogging, surface roughness and membrane fouling. Therefore, the functional materials should be evenly distributed in positions that the water flow can reach as much as possible, while ensuring that the fillers are firmly bound to the membrane material to reduce particle shedding. The binding between filler and membrane can be improved by polydopamine (PDA) bonding, silane coupling, surface amination or in-situ growth.

5.2. Influence of water quality and matrix factors

pH changes the charged state of pollutants and the membrane surface, thereby affecting filtration and adsorption. For PFAS, under acidic conditions, the amine groups in polyethyleneimine (PEI) are more likely to be positively charged, which can enhance the adsorption of negatively charged PFAS. He Kunzhen et al. found that acidic conditions are favorable for PFOA adsorption [12]; the studies of Fujioka et al. and Zhi et al. also showed that the membrane surface charge affects the filtration of PFAS. The situation of antibiotics is more complex; different antibiotics may be positively charged, negatively charged or nearly neutral at different pH, so electrostatic attraction or repulsion may occur between them and the membrane, which in turn changes the filtration and adsorption effects.

Natural organic matter (NOM) also affects the removal of PFAS and antibiotics by the membrane. On the one hand, NOM can compete with pollutants for the adsorption sites on the membrane surface and nanomaterials, reducing the sites that can actually adsorb PFAS and antibiotics; on the other hand, NOM may also form a fouling layer on the membrane surface and clog part of the membrane pores, thereby changing the filtration effect. Gagliano et al. pointed out that NOM reduces the adsorption capacity of materials for short-chain PFAS [8]. Therefore, in real water bodies, the removal of pollutants by the membrane is usually obviously affected by NOM.

Coexisting ions in water such as Ca2+ and Mg2+ also affect filtration and adsorption. These ions may change the charge action on the membrane surface, and may also compete with pollutants for adsorption sites, thereby affecting the interaction between pollutants and the membrane. He Kunzhen et al. found that multiple coexisting ions inhibit PFOA adsorption. Nian Qixun found in the experiment of antibiotic adsorption by the MOF-801@PDA@PAN nanofiber membrane that as the NaCl concentration increased, the adsorption efficiency of many antibiotics gradually decreased; after MgCl2 was added, the adsorption efficiency dropped even more obviously, showing that coexisting ions interfere with the electrostatic interaction between the membrane material and antibiotics. Therefore, even if the membrane itself has many adsorption sites, the actual adsorption effect may decrease in complex water bodies due to the influence of coexisting ions.

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When PFAS and antibiotics coexist, competition may also occur between the two types of pollutants. Different pollutants will preferentially occupy the adsorption sites that better match their own structures; for example, long-chain PFAS more easily interact with hydrophobic sites, while antibiotics containing aromatic rings or able to bind metals more easily occupy the corresponding adsorption sites. In this way, the presence of one pollutant may affect the adsorption and filtration of the other. Therefore, in real water bodies, it is necessary to consider at the same time the effects of pH, natural organic matter, coexisting ions and the coexistence of multiple pollutants on the adsorption-filtration process.

5.3. Influence of process operation parameters

Transmembrane pressure and water flow velocity directly affect the filtration and adsorption processes of nanocomposite membranes. Appropriately increasing the pressure can increase the water flux and let more water pass through the membrane, but when the pressure is too high, the residence time of pollutants in the membrane is shortened and the chance of contacting adsorption sites is reduced. For membranes dominated by filtration, appropriately increasing the pressure is favorable for water production; for membranes that also rely on adsorption to remove pollutants, water flux and adsorption time need to be balanced. The dynamic membrane studies of Bi et al. and Wan et al. showed that both the water flow velocity and the residence time of pollutants in the membrane affect the final removal effect.

Cleaning cycles and regeneration times also affect the long-term operation of nanocomposite membranes. As the filtration time extends, pollutants gradually accumulate on the membrane surface and in the membrane pores, causing the water flux to decline, and part of the adsorption sites is also occupied. Therefore, backwashing, chemical cleaning or other methods are needed to periodically remove the pollutants on the membrane surface so that the filtration performance is restored. For nanocomposite membranes with adsorption functions, regeneration is also needed to make the occupied adsorption sites function again. Nian Qixun's research showed that the adsorption material can still maintain a certain removal capacity after multiple regenerations. Therefore, reasonably controlling the cleaning cycle and regeneration times is conducive to maintaining both the filtration capacity and the adsorption capacity of the membrane.

Temperature and operation time also affect pollutant removal. Increasing the temperature can speed up the movement and diffusion of pollutants in water, but the influence of temperature on different adsorption actions is not exactly the same. As the operation time extends, the adsorption sites in the membrane will be gradually occupied by pollutants, and the adsorption speed and adsorption capacity may decline accordingly. Nian Qixun's adsorption kinetics research showed that the time needed for different antibiotics to reach adsorption equilibrium differs. Therefore, during continuous operation, nanocomposite membranes need to consider the water flow velocity, the contact time between pollutants and adsorption sites, and the gradual occupation of adsorption sites at the same time.

6. Current bottlenecks and problems

From all the above analyses it can be seen that nanocomposite membranes are expected to use the joint action of filtration and adsorption to remove PFAS and antibiotics from water at the same time. Among them, membrane pores and surface charge can play a filtering role, and different functional materials can provide adsorption sites for PFAS and antibiotics, so the two have the possibility of combination in structure and mode of action. However, the conclusions of this paper on the

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simultaneous removal of PFAS and antibiotics are mainly inferred from filtration and adsorption studies in different literature, and studies directly targeting the same nanocomposite membrane under PFAS-antibiotic coexistence conditions are still few at present. In addition, the studies cited in this paper include both static adsorption experiments and continuous filtration experiments, and the membrane materials, pollutant concentrations and operating conditions used in different studies are not exactly the same, so some experimental results cannot be directly compared. The filtration-promoting-adsorption and adsorption-strengthening-filtration proposed in this paper can explain the possible synergistic effect of nanocomposite membranes, but whether PFAS and antibiotics compete for membrane pores and adsorption sites when coexisting, and whether this synergy can be maintained during long-term continuous operation, cannot yet be concluded from the existing literature alone. Therefore, the results of this paper mainly show the theoretical feasibility and possible mechanisms of using the same nanocomposite membrane to achieve synergistic adsorption-filtration removal of PFAS and antibiotics, and the actual removal effect still needs further experimental verification.

7. Conclusions and prospects

The future design of nanocomposite membranes should further take into account both the filtration and adsorption of PFAS and antibiotics. The filtration effect can be improved by adjusting the membrane pore size and surface charge, and positively charged, hydrophobic, aromatic structures and metal sites can be set in the membrane so that PFAS and antibiotics of different structures can all be adsorbed. The amount and distribution of functional materials should also be reasonably controlled to avoid problems such as particle aggregation, membrane pore clogging and embedding of adsorption sites.

Future experimental studies need to use more collected natural raw water for dynamic continuous filtration tests, and consider the situation where PFAS and antibiotics coexist. Real water also contains natural organic matter and various ions, and these substances may affect filtration and adsorption. Therefore, further research is needed on whether competition occurs when different pollutants coexist, and whether nanocomposite membranes can maintain good filtration and adsorption capacity under continuous operation.

In addition, the reusability and long-term operation capability of nanocomposite membranes need to be improved. In-situ cleaning, regeneration or adding catalytic and self-cleaning functions to the membrane can be used to further remove the adsorbed pollutants and make the adsorption sites function again. At the same time, the stability and preparation process of membrane materials should be further improved, so that adsorption-filtration synergy membranes can gradually move from laboratory research to practical water treatment applications.

8. References

[1] Li, J., Zhang, H. D., Wang, X. B., et al. (2024). Research progress on analytical methods for per- and polyfluoroalkyl substances in the environment. *Chemical Reagents, 46*(11), 17–26.

[2] Crone, B. C., Speth, T. F., Wahman, D. G., et al. (2019). Occurrence of per- and polyfluoroalkyl substances (PFAS) in source water and their treatment in drinking water. *Critical Reviews in Environmental Science and Technology, 49*(24), 2359–2396.

[3] Ateia, M., Maroli, A., Tharayil, N., et al. (2019). The overlooked short- and ultrashort-chain poly- and perfluorinated substances: A review. *Chemosphere, 220*, 866–882.

[4] Qi, Y. B., Zhang, S. J., Meng, X. R., et al. (2021). Current status and research progress of antibiotic wastewater treatment technology. *Applied Chemical Industry, 50*(9), 2587–2593+2597.

DOI: 10.54254/2755-2721/2027.AD38205

[5] Wu, X. J., Shi, G. J., & Wang, Y. Y. (2022). Effects of microplastics on the spread and horizontal gene transfer of antibiotic resistance genes. *China Environmental Science, 42*(8), 3957–3968.
[6] Zhang, Y. H., Huang, T. C., Jiang, S. C., et al. (2023). Research progress on membrane technology for antibiotic wastewater treatment from livestock and poultry. *Ion Exchange and Adsorption, 39*(1), 87–96.
[7] Das, S., & Ronen, A. (2022). A review on removal and destruction of per- and polyfluoroalkyl substances (PFAS) by novel membranes. *Membranes*.
[8] Gagliano, E., Sgroi, M., Falciglia, P. P., et al. (2020). Removal of poly- and perfluoroalkyl substances (PFAS) from water by adsorption: Role of PFAS chain length, effect of organic matter and challenges in adsorbent regeneration. *Water Research, 171*, 115381.
[9] Geng, Q. W., Ban, Y. H., Zhang, J. D., et al. (2024). Preparation methods of metal-organic framework/polymer composites. *Ion Exchange and Adsorption, 40*(3), 196–209.
[10] Lu, H., Yang, Q., & Kong, Y. (2023). Research progress on adsorption removal and oxidative degradation of organic pollutants in water by metal-organic framework materials. *Materials Reports, 37*(4), 170–182.
[11] Fujioka, T., Takeuchi, H., Tahara, H., et al. (2024). Effects of functional groups of polyfluoroalkyl substances on their removal by nanofiltration. *Water Research X*, 100233.
[12] He, K. Z., Liu, Y., Xing, X., et al. (2026). Study on the adsorption performance of PAN/PEI nanofiber membranes for PFOA in water. *China Environmental Science, 46*(2), 809–820.
[13] Bi, Y., Meng, X., Tan, Z., et al. (2024). A novel ZIF-L/PEI thin film nanocomposite membrane for removing perfluoroalkyl substances (PFASs) from water: Enhanced retention and high flux. *Science of the Total Environment, 925*, 171727.
[14] Zhi, Y., Zhao, X., Shuai, A., et al. (2025). Enhancing rejection of short-chain per- and polyfluoroalkyl substances by tailoring the surface charge of nanofiltration membranes. *Water Research, 272*, 122931.
[15] Wang, Y. J., Zhou, Z. A., Feng, W. Y., et al. (2026). Research progress on removal of typical antibiotics from water by iron-based metal-organic frameworks (Fe-MOFs). *Technology of Water Treatment, 52*(2), 34–40.
[16] Zhao, F. M., Zhang, Y., Sun, W. J., et al. (2020). Research progress on adsorption removal of antibiotic pollutants from water by activated carbon. *Ion Exchange and Adsorption, 36*(2), 182–192.
[17] Wang, X. F., Zhang, S., Liu, J. Z., et al. (2021). Fe3O4@reduced graphene oxide nanocomposite and its adsorption of tetracycline antibiotics. *Ion Exchange and Adsorption, 37*(1), 76–87.
[18] Nian, Q. X. (2025). *Development and application of nanofiber membranes for efficient antibiotic adsorption* [Doctoral dissertation, Southeast University].
[19] Cevallos-Mendoza, J. E., Alay-Macias, G., Figueira, F., et al. (2024). Nanocomposite HKUST-1@polysulfone membrane for the adsorptive removal of tetracyclines in waters. *Separation and Purification Technology, 330*, 125568.
[20] Wan, H., Fang, F., Shi, K., et al. (2024). Dual-functional adsorptive membranes for PFAS removal: Mechanism, CFD simulation, and selective enrichment. *Chemical Engineering Journal, 500*, 156095.
[21] Chen, Y. A., Geng, Q. W., Cao, X. H., et al. (2023). Challenges and latest strategies for industrial application of metal-organic framework materials. *Ion Exchange and Adsorption, 39*(1), 75–86.