Review paper

Structure-Performance Relationships in Nanofiltration Membranes: From Molecular Architecture to Intelligent Membrane Systems

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Abstract: Nanofiltration (NF) has become an indispensable platform for sustainable separations, yet its continued advancement is constrained by persistent trade-offs between permeability and selectivity, limited solute-solute discrimination, fouling susceptibility, and poor long-term stability under aggressive operating conditions. Despite rapid progress across polyamide chemistry, nanomaterial incorporation, and process modelling, the field remains fragmented, with insights confined to isolated material classes, fabrication routes, or applications, and lacking a unifying framework that connects molecular design to system-level performance. This review addresses that gap by establishing a coherent, multiscale structure–performance framework that traces a continuous mechanistic thread from molecular architecture to industrial module. We first critically examine the molecular-scale design of polyamide selective layers, questioning whether it genuinely reshapes membrane structure and introduces functional engineered nanoscale transport pathways. We then analyse morphology-performance correlations, advanced multiscale predictive modelling, and the rapidly emerging role of artificial intelligence and data-driven design in accelerating membrane discovery and optimization. Beyond material performance, we critically appraise fouling mechanisms and antifouling strategies, sustainability through life-cycle and techno-economic assessment, and the frequently underappreciated

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lab-to-module performance gap that governs real-world deployment. Throughout, we interrogate conflicting findings, reproducibility and scalability limitations, and the economic and environmental barriers that separate laboratory achievements from industrial reality. By integrating these traditionally siloed domains within a single critical synthesis, this review consolidates fragmented knowledge, identifies the most consequential research gaps, and articulates a scientific roadmap toward highly selective, energy-efficient, and industrially viable NF systems for global water security and sustainable resource recovery.

Keywords: Nanofiltration, Polyamide thin-film composite membranes, Morphology-performance relationships, Data-driven membrane design, Laboratory-to-module scale-up, Membrane sustainability

1. Introduction

Nanofiltration (NF) has emerged as one of the most versatile and energy-efficient pressure-driven separation technologies in modern membrane science, occupying a strategic niche between reverse osmosis (RO) and ultrafiltration and playing an increasingly critical role in addressing global challenges related to water scarcity, wastewater treatment, resource recovery, and sustainable chemical processing [1, 2]. NF membranes typically exhibit pore sizes in the range of 1-2nm and molecular weight cut-offs of 200-1000 Da, enabling the selective rejection of multivalent ions, organic molecules, and micropollutants while permitting the partial permeation of monovalent salts and water [3]. This distinctive combination of moderate selectivity and low operating pressures (5–20 bar) underpins the appeal of NF as an enabling technology for desalination, pharmaceutical purification, dye–salt fractionation, and the recovery of critical metals [4].

The development of NF membranes has been driven by successive efforts to overcome the limitations of earlier membrane materials and architectures. The earliest pressure-driven desalination membranes were based on asymmetric cellulose acetate (CA), pioneered by Loeb and Sourirajan in the 1950s–1960s [5]. Although these membranes demonstrated the feasibility of membrane-based desalination, their practical application was constrained by relatively low water permeability, a narrow operating pH range, and limited chemical and thermal stability. A major breakthrough came with the development of polyamide thin-film composite (PA-TFC) membranes by Cadotte and co-workers in the 1970s through interfacial polymerization (IP) [6, 7]. By decoupling the selective and mechanical functions of the membrane, this architecture enabled the formation of an ultrathin polyamide selective layer on a porous, non-selective substrate, with the selective layer typically having a thickness of tens to hundreds of nanometres and the supporting substrate providing the necessary mechanical strength [8]. This architectural innovation substantially improved water permeability, separation performance, and operational stability compared with earlier cellulose-based membranes and established PA-TFC membranes as the dominant platform for modern NF and RO applications.

Subsequent advances in polyamide chemistry have enabled progressively finer control over selective-layer structure and molecular separation behaviour. The substitution of aromatic diamines with piperazine (PIP), for example, produces looser, semi-aromatic networks with larger effective free volume, thereby favouring higher water permeability and preferential rejection of divalent ions, which is characteristic of commercial NF membranes [9]. Over the past two decades, this design space has expanded considerably through rational monomer engineering, including the development of novel and mixed-monomer systems [10, 11], the incorporation of functional moieties (carboxylic, zwitterionic, and sulfonic groups), and the use of macrocyclic building blocks. Beyond monomer chemistry, refined control over the interfacial polymerization (IP) process through manipulation of monomer partitioning and diffusion has enabled increasingly precise regulation of selective-layer thickness, cross-linking density, and surface morphology [12–14].

A more recent frontier has been the integration of nanomaterials into TFC and mixed-matrix membrane (MMM) architectures, where embedded or interfacially incorporated nanomaterials are exploited to restructure the selective layer and introduce engineered molecular transport pathways. Rather than acting as inert additives, these nanomaterials can reshape membrane architecture across multiple length scales by modifying free-volume distribution, interfacial cross-linking, and surface morphology, thereby directly influencing the structure-transport-performance relationships that govern next-generation NF membranes. The porous and crystalline frameworks of metal-organic frameworks (MOFs) and covalent organic frameworks (COFs) furnish well-defined, sub-nanometre intrinsic channels that can facilitate rapid, size- and charge-selective water and ion transport, potentially mitigating the conventional permeability–selectivity trade-off [15]. Two-dimensional laminates such as graphene oxide (GO) and MXenes create tortuous interlayer nanochannels who’s spacing and surface chemistry can be tuned to

sieve ions and small molecules [16–18], while ionic liquids (ILs) modulate interfacial polymerization and impart tailored polarity and charge to the resulting network [19]. Collectively, these strategies aim to establish preferential, low-resistance transport corridors that circumvent the diffusion-limited pathways of dense polyamide, thereby providing a potential mechanistic route to mitigate the permeability–selectivity trade-off.

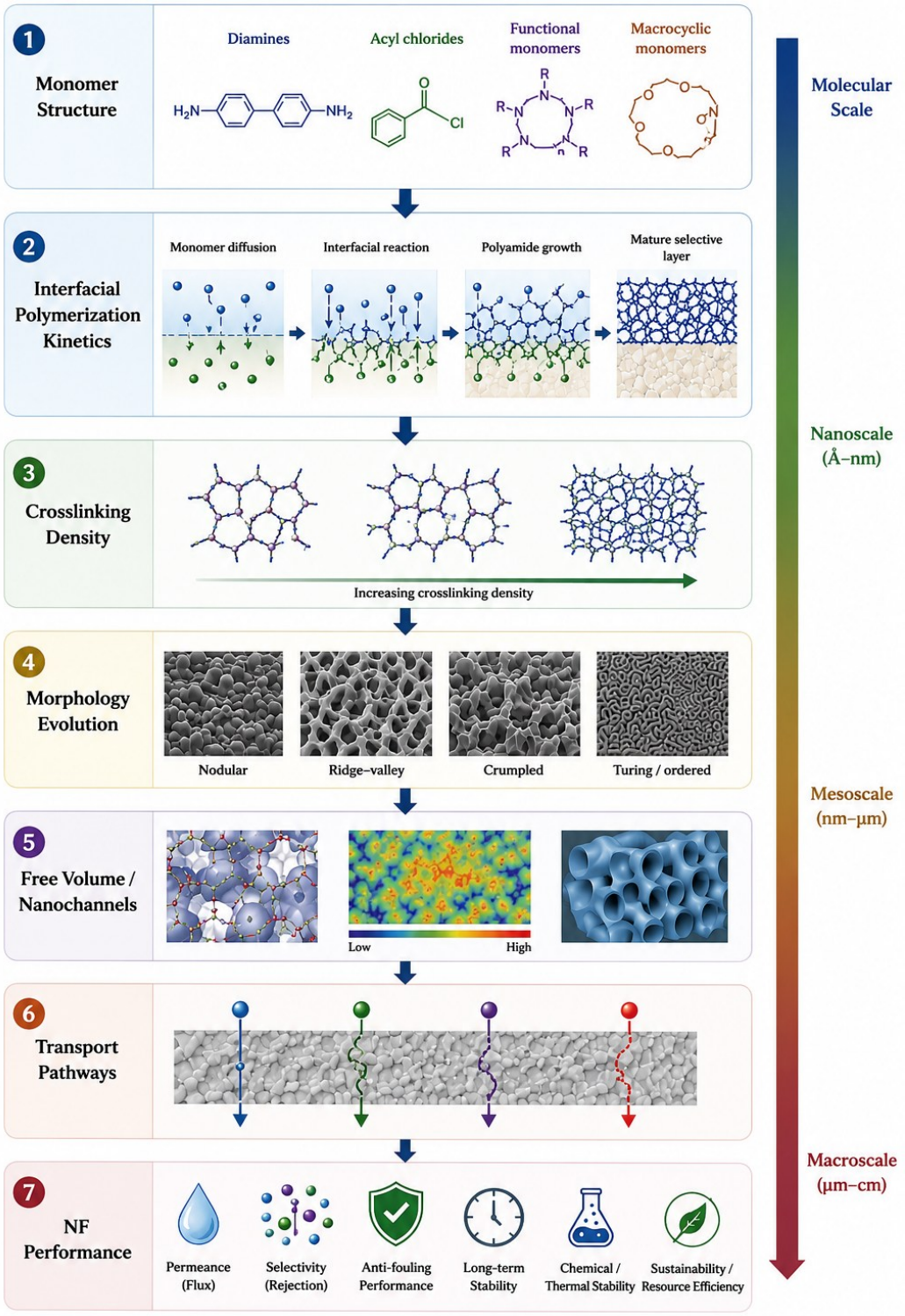

Figure 1. Schematic illustration of the multiscale structure-transport-performance evolution in next-generation NF membranes.

However, the reported benefits of these strategies must be interpreted with caution. Much of the TFC and functional-monomer literature reports substantial permeability or selectivity gains under idealized, short-duration laboratory conditions, yet the reproducibility, long-term stability, and scalability of these enhancements remain inadequately established. Nanofiller-based membranes, in particular, are frequently undermined by poor polymer–filler interfacial compatibility, non-uniform dispersion, and interfacial defect formation, which can generate non-selective transport pathways that erode rejection over time or upon aging. Divergent and occasionally contradictory performance data across studies employing nominally identical materials often reflect differences in filler loading, dispersion protocols, substrate characteristics, and testing conditions rather than intrinsic material superiority, with such discrepancies seldom being systematically deconvoluted. Moreover, the economic viability, environmental footprint, and industrial manufacturability of many advanced nanomaterials remain largely unaddressed, leaving a considerable gulf between the performance claimed at bench scale and that which is demonstrably realizable in practice.

Consequently, despite these impressive advances, several deep-seated challenges continue to constrain state-of-the-art NF membranes. Foremost among these is the persistent permeability–selectivity trade-off, which fundamentally limits simultaneous gains in flux and rejection. Additional unresolved issues include pronounced fouling susceptibility, insufficient solute–solute selectivity for the precise separation of similarly sized species—an increasingly critical requirement for resource recovery and ion fractionation, and limited long-term stability under harsh conditions such as extreme pH, elevated temperature, or exposure to aggressive organic solvents [20, 21]. Addressing these challenges demands a rigorous, mechanistically grounded understanding of the material chemistry and molecular design principles governing selective-layer formation, coupled with a clear elucidation of the transport phenomena that dictate permeability and selectivity, and increasingly, the integration of these insights with computational and artificial intelligence (AI)-driven design tools. Yet the existing review literature, while extensive, remains conspicuously fragmented: individual reviews typically address isolated facets of the field, such as new materials, surface modification, or application-specific performance, without reconciling these dimensions within a coherent conceptual framework spanning the molecular, materials, computational, and systems-level scales that collectively determine membrane behaviour.

To bridge this gap, the present review establishes a unified, multiscale structure–performance framework for NF membranes. Rather than treating emerging materials, computational approaches, and engineering considerations as independent research directions, this review examines how structural features at different length scales govern membrane formation, transport behaviour, stability, and practical performance. Specifically, we trace the evolution of structure-performance relationships from molecular architecture and polyamide chemistry through interfacial polymerization, nanoscale morphology regulation, and transport modelling to AI-assisted prediction. Furthermore, fouling behaviour, sustainability, and module-scale implementation are discussed as critical performance constraints that determine whether laboratory-scale structural innovations can be translated into practical membrane systems. By integrating these interconnected perspectives and critically evaluating current limitations, contradictory findings, and unresolved challenges, this review aims to provide a mechanistic roadmap for the rational design of highly selective, stable, scalable, and sustainable NF membranes for advanced separations and water treatment applications.

2. Molecular Architecture of Polyamide Selective Layers: A Multiscale Perspective

The structure and separation performance of PA-TFC membranes are governed by a hierarchical sequence of events extending from molecular-scale monomer selection to macroscopic operational performance. Molecular architecture determines interfacial polymerization (IP) kinetics, this kinetics regulate cross-linking density, free-volume distribution, and nanoscale transport pathways and the resulting network evolves into mesoscale morphologies that ultimately influence permeance, selectivity, fouling behaviour, stability, and process viability. Figure 1 provides a conceptual representation of this multiscale cascade, linking monomer structure, reaction-diffusion control, cross-linking density, morphology evolution, free volume/nanochannels, transport pathways, and NF performance.

Importantly, Figure 1 should be regarded as a framework for understanding causal connections across scales rather than as evidence that a single design variable can independently determine membrane performance. For example, increased free volume may enhance water transport only when it is spatially controlled and integrated into selective pathways, otherwise, it can generate non-selective defects. Likewise, highly crumpled morphologies may increase effective surface area and permeance but may also introduce structural heterogeneity, fouling-prone recesses, or mechanical instability. The discussion below therefore evaluates

molecular design strategies not only according to reported performance gains, but also according to their underlying mechanisms, trade-offs, reproducibility, long-term stability, and potential for industrial translation.

2.1 Monomer Structure as the Primary Design Variable

At the molecular scale, the chemical composition and topology of the PA selective layer are primarily determined by the aqueous-phase amine and organic-phase acyl chloride monomers. Conventional systems based on piperazine (PIP) or *m*-phenylenediamine (MPD) and trimesoyl chloride (TMC) remain the principal reference platforms for NF and reverse osmosis membrane fabrication. These systems illustrate the fundamental relationship between monomer structure and network architecture: MPD-TMC typically forms highly cross-linked and densely packed aromatic PA networks, whereas PIP-TMC generally produces more flexible and less densely cross-linked semi-aromatic structures [22]. Consequently, MPD-derived networks tend to favour tighter solute rejection, while PIP-derived networks often provide higher water permeance and stronger preferential rejection of divalent ions. These contrasting behaviours reflect the persistent permeability-selectivity trade-off that continues to define PA membrane design.

Recent research has substantially expanded the available monomer-design space through alcohol-, phenol-, and amine-based monomers, as well as functionalized monomers bearing carboxylic, sulfonic, quaternary ammonium, and zwitterionic groups [23]. These monomers are intended to modify intermolecular interactions, monomer reactivity, surface charge, hydrophilicity, and fractional free volume (FFV). In parallel, macrocyclic monomers, including cyclodextrins, calixarenes, pillar[n]arenes, and crown ethers, introduce shape-persistent cavities that may act as pre-organized free-volume elements or selective transport sites [24, 25].

The mechanistic appeal of molecular design lies in its potential to control both network densification and molecular transport. Monomer geometry, including linear, planar, non-planar, and three-dimensional configurations, affects steric packing, diffusion behaviour, and cross-linking potential. Higher monomer functionality generally provides additional reactive sites and can promote a more densely cross-linked network with smaller effective pores. Conversely, non-planar, bulky, or rigid monomers may disrupt efficient chain packing and promote greater free-volume connectivity [26 - 28]. The resulting effect is not inherently beneficial or detrimental, controlled free volume can facilitate water transport, whereas excessive steric disruption may broaden the pore-size distribution or generate weakly cross-linked regions that reduce selectivity.

Accordingly, the superiority of a particular monomer cannot be inferred solely from an increase in water permeance or salt rejection. In many studies, changes in monomer chemistry occur simultaneously with changes in solvent composition, monomer concentration, substrate properties, reaction time, or post-treatment conditions. The reported performance difference may therefore arise from a combined effect of molecular structure and processing conditions rather than from monomer chemistry alone. This issue complicates direct comparison among studies and limits the development of universal structure-property relationships.

A further limitation is that many advanced monomers are evaluated predominantly under short-duration laboratory conditions using model salts or single-solute feeds. Such tests provide valuable proof of concept but do not establish whether the resulting network remains stable under sustained pressure, complex feed compositions, chemical cleaning, or variable pH and ionic strength. The synthesis complexity, purification requirements, commercial availability, and cost of advanced functional or macrocyclic monomers also require consideration. A molecular architecture that delivers high initial performance but cannot be reproducibly synthesized, scaled, or incorporated into established membrane-manufacturing processes may have limited practical relevance. Future monomer design should therefore be evaluated against conventional MPD–TMC and PIP–TMC benchmarks under comparable fabrication and testing conditions, while incorporating durability, reproducibility, and manufacturability into the definition of performance.

2.2 Interfacial Polymerization Kinetics, Cross-Linking Density, and Free-Volume Engineering

The molecular characteristics of the monomers are translated into nanoscale PA architecture through IP. As illustrated in Figure 1, IP is governed by coupled diffusion-reaction phenomena in which aqueous-phase amines diffuse toward the organic interface

and react rapidly with acyl chlorides to form an ultrathin PA selective layer [2]. Because the reaction is fast, the initially formed PA layer progressively restricts monomer transport and creates a self-limiting growth process. The final membrane structure is therefore determined not only by the identities of the monomers but also by their diffusion rates, interfacial partitioning, local stoichiometry, reaction kinetics, and the evolving barrier imposed by the growing PA film.

This dynamic process can generate structural heterogeneity through the thickness of the selective layer. During the early stage of IP, rapid reaction may produce a dense and highly cross-linked region near the organic-facing interface. As film growth proceeds, transport resistance increases and the reaction becomes more diffusion-limited, potentially generating less densely cross-linked regions closer to the aqueous phase. Such heterogeneity can be advantageous if dense domains provide effective molecular sieving while less dense but controlled regions facilitate water transport. However, if the distribution of cross-linking density and free volume becomes uncontrolled, the same heterogeneity can lead to broad pore-size distributions, non-selective pathways, and reduced rejection.

Cross-linking density is therefore a central parameter linking molecular design to separation performance. It controls chain connectivity, interchain spacing, pore dimensions, FFV, and the balance between permeance and selectivity. Higher cross-linking density generally produces a tighter network with lower FFV and higher solute rejection, but also increases resistance to water transport. Lower cross-linking density can increase FFV and water permeability, but may compromise selectivity if transport occurs through poorly controlled regions. The relationship is further complicated by monomer geometry. Higher-functionality monomers may increase the number of cross-linking points, whereas steric hindrance associated with non-planar or macrocyclic structures can limit chain packing and promote free-volume formation [28].

Functionalized monomers can also influence cross-linking density indirectly by modifying monomer diffusion, interfacial reactivity, and electrostatic interactions. Such strategies may enable thinner and more porous active layers [29]. However, the distinction between beneficial free-volume engineering and defect generation remains insufficiently resolved. High FFV is desirable only when voids are narrowly distributed, molecularly selective, and sufficiently stable during operation. By contrast, excessive or poorly controlled FFV can create non-selective leakage pathways. Because conventional permeance and salt-rejection measurements cannot independently distinguish controlled nanochannels from defects, claims of trade-off mitigation should be interpreted cautiously unless accompanied by rigorous structural characterization and long-term stability assessment.

Beyond intrinsic monomer design, cross-linking density can be regulated through additives that modify monomer diffusion, interfacial structure, and local stoichiometry [30]. Interfacial regulators, including surfactants, cosolvents, bio-derived additives, and nanomaterials, can influence aqueous-phase transport and therefore provide an effective route to kinetic control [31].

These strategies demonstrate that IP can be manipulated beyond conventional monomer concentration control. Nevertheless, additive-mediated IP also presents significant limitations. The outcome is often highly sensitive to additive loading, dispersion, monomer purity, substrate morphology, temperature, humidity, and mixing conditions. Minor variation in any of these parameters can alter the reaction-diffusion balance and thereby influence thickness, cross-linking density, morphology, and defect formation. This sensitivity may contribute to inconsistent performance among nominally similar membranes and creates challenges for batch-to-batch reproducibility. The scale-up of such approaches is also uncertain because controlling interfacial composition and reaction uniformity over large membrane areas is inherently more difficult than in laboratory-scale flat-sheet fabrication.

Moreover, most studies report initial separation performance without systematically examining compaction, hydrolytic aging, chemical cleaning, or prolonged exposure to realistic feed compositions. Additives that increase permeance by suppressing dense polymer growth or increasing free volume may also increase vulnerability to structural rearrangement or defect formation during long-term operation. The environmental and economic implications of specialized surfactants, nanomaterials, and additives are similarly insufficiently established. Thus, the principal unresolved challenge is to convert empirical kinetic control into predictive design. Integrating computational techniques such as density functional theory (DFT), molecular dynamics (MD), artificial intelligence (AI) and complementary experimental characterizations could clarify how monomer chemistry, additive interactions,

diffusion, and reaction pathways control network formation. Such a framework is needed to develop ultrathin PA layers that combine high performance with reproducibility, durability, and industrial manufacturability.

2.3 Morphology Evolution and Structure-Transport Relationships

The nanoscale processes of IP, cross-linking, and free-volume formation are expressed at the mesoscale through selective-layer morphology. Figure 1 depicts a progression from nodular to ridge-and-valley, crumpled, and Turing-type ordered structures. These morphologies influence effective surface area, local diffusion distance, thickness distribution, transport-pathway connectivity, mechanical response, and fouling behaviour. They are therefore not merely visual features of PA layers but structural determinants of membrane performance.

Nodular morphologies are often associated with relatively slow or low-concentration IP conditions and consist of dense quasi-spherical aggregates. Ridge-and-valley morphologies are characteristic of many conventional NF and reverse osmosis membranes and emerge through non-uniform polymer growth, interfacial instability, differential swelling, and post-treatment relaxation. Crumpled and folded architectures have attracted increasing attention because they can increase effective filtration area and reduce local transport resistance. Sub-10 nm PA nanofilms with tunable crumpled morphologies have been fabricated, achieving ultrahigh solvent permeance (>100 L m^{-2} h^{-1} bar^{-1}) while retaining high solute rejection; permeance increased with the degree of crumpling [32]. Turing-type structures were generated by suppressing aqueous-phase monomer diffusion, producing nanoscale heterogeneous domains with enhanced transport [33]. Similarly, lignin-derived additives promoted monomer partitioning and interfacial instability, producing ultrathin, highly cross-linked, crumpled PA layers with high permeance (~26 L m^{-2} h^{-1} bar^{-1}) and strong ion selectivity [12].

Other approaches, including nanoparticle sacrificial templates [34], MXene-assisted IP [35], and scaffold-confined polymerization [36], demonstrate that spatial confinement and transport regulation can induce high-area selective-layer architectures with permeance exceeding ~50 L m^{-2} h^{-1} bar^{-1} while maintaining high rejection. The formation of these structures is governed by coupled physicochemical phenomena, including reaction-diffusion instability, localized heating from the exothermic IP reaction, temperatures approaching ~90 °C, nanobubble formation, gas evolution, and structural relaxation during post-treatment [37].

Although morphology engineering is frequently presented as a route to overcome the permeability-selectivity trade-off, the available literature indicates that its effects are not universal. Reported permeance values vary substantially, from approximately 26 to >100 L m^{-2} h^{-1} bar^{-1}, even among membranes described as crumpled or highly ordered [38]. These discrepancies likely reflect differences in monomer chemistry, additive type, substrate morphology, selective-layer thickness, extent of cross-linking, effective-area estimation, feed composition, and operating pressure. Consequently, morphology alone cannot be regarded as an independent predictor of separation performance. A highly crumpled layer may exhibit high permeance because of increased surface area, but it may also contain thinner regions, less cross-linked domains, or defects that contribute to transport.

Morphology also introduces potential operational disadvantages. Rough ridge-and-valley and crumpled surfaces can increase effective membrane area and water flux, but recessed features may retain foulants, promote concentration polarization, and reduce cleaning efficiency. By comparison, smoother nodular or highly ordered surfaces may be less susceptible to particulate deposition but may provide lower accessible area and reduced permeance. The mechanical integrity of high-aspect-ratio folds and ridges during long-term pressurization, chemical cleaning, and repeated operating cycles is also insufficiently established. Compaction, structural relaxation, or collapse of fragile morphological features could reduce the initial flux advantage over time.

Future morphology engineering should therefore be evaluated using criteria that extend beyond initial flux and rejection. The most relevant metrics include surface-area normalization, selective-layer integrity, fouling propensity, cleaning recovery, mechanical stability, compaction resistance, and module-scale hydrodynamics. The field would benefit from standardized methods for reporting morphology, effective filtration area, thickness distribution, and long-term performance to enable meaningful comparison between crumpled, Turing-type, and conventional PA architectures.

2.4 From Molecular Transport Pathways to System-Level NF Performance

The structural features discussed above ultimately determine membrane performance through their influence on molecular transport pathways. As conceptually illustrated in Figure 1, free volume and nanochannels represent the intrinsic void space generated within the PA matrix by monomer geometry, cross-linking density, and chain packing, whereas transport pathways refer to the connected routes through which water and solutes traverse the selective layer. Although these concepts are closely related, they are not equivalent. A membrane may possess substantial local free volume without exhibiting high permeance if these voids are isolated, inaccessible, or highly tortuous. Conversely, highly connected pathways can enhance water transport but may compromise solute rejection when they arise from poorly cross-linked regions or non-selective defects rather than from controlled molecular channels.

In dense PA domains, transport is predominantly governed by solution-diffusion, molecular sieving, and charge-based exclusion. High cross-linking density reduces interchain spacing and restricts solute transport, thereby improving rejection but increasing hydraulic resistance. In contrast, less densely packed regions may contain interchain gaps, nanochannels, or cavity-derived pathways that reduce resistance to water transport. Accordingly, molecular functionalization, macrocyclic design, free-volume engineering, and morphology regulation all pursue a common objective: to create continuous, low-tortuosity, and molecularly selective pathways that facilitate water permeation without opening non-selective routes for ions or organic solutes.

This objective, however, remains difficult to achieve reproducibly. An increase in permeance may reflect genuinely selective nanochannels, but it may also originate from a reduced active-layer thickness, increased effective surface area, incomplete cross-linking, or defect formation. These mechanisms cannot be distinguished reliably from permeance and rejection values alone. Therefore, claims that a particular molecular or morphological strategy has overcome the permeability-selectivity trade-off should be interpreted cautiously unless supported by complementary evidence linking chemical structure, free-volume distribution, transport-pathway connectivity, and separation behaviour. More rigorous integration of molecular simulation, nano structural characterizations, transport experiments, and long-term filtration tests is needed to establish whether the proposed pathways remain selective and stable during operation.

The consequences of these transport characteristics become evident at the macroscale, where membrane performance is assessed not only by permeance and solute rejection but also by fouling resistance, chemical and thermal stability, mechanical robustness, and sustainability. For instance, high fractional free volume, ultrathin selective layers, and crumpled morphologies can increase permeance, with selected architectures exceeding 50-100 L m^{-2} h^{-1} bar^{-1} [12]. At the same time, selectivity depends on the uniformity of pore-size distribution, the degree of cross-linking, membrane charge, and the accessibility of selective transport pathways. Similarly, macrocyclic monomers containing sub-nanometre cavities can provide strong mono/divalent-ion discrimination [25] while charged and hydrophilic functional groups can influence ion partitioning and foulant-surface interactions [39, 40]. These results demonstrate the potential of molecular architecture to tailor NF performance; however, they also illustrate that improvements in one metric may impose penalties in another. For example, increased free volume can promote permeance but weaken rejection or structural stability, while rough and highly permeable morphologies can increase flux but intensify fouling or concentration polarization.

This trade-off becomes even more consequential during the transition from laboratory-scale membrane coupons to practical membrane modules. High intrinsic permeance does not necessarily translate into lower process energy consumption or improved product quality. At the module scale, concentration polarization, pressure losses, spacer geometry, flow distribution, feed variability, fouling, compaction, cleaning frequency, and membrane replacement intervals can strongly influence overall separation efficiency. A membrane that performs exceptionally under pure-water or single-salt testing may exhibit a more limited advantage when operated with realistic multicomponent feeds. Likewise, a rough or highly porous selective layer may provide high initial flux but incur greater operational penalties if it accelerates foulant accumulation or requires more frequent cleaning.

Accordingly, the evaluation of emerging PA architectures must extend beyond initial water permeance and solute rejection. Meaningful assessment should include fabrication yield and batch-to-batch reproducibility, long-term hydraulic and chemical

stability, fouling reversibility, mechanical integrity, compatibility with spiral-wound or hollow-fibre module fabrication and life-cycle implications. In this context, Figure 1 is not merely a structure-performance map; it also represents a bidirectional design framework. Bottom-up control of monomer chemistry, IP kinetics, cross-linking, and morphology must be guided by top-down requirements for separation quality, energy consumption, membrane lifetime, manufacturability, and environmental performance. Only through such coordinated multiscale optimization can high-performing PA selective layers progress from laboratory demonstrations to durable, scalable, and industrially deployable NF systems.

Although intrinsic molecular design and IP control provide the foundation for tailoring PA transport pathways, polymer-chain packing and network stability impose practical limits on the extent to which these strategies can independently optimise NF performance. This limitation has motivated nanostructuring and filler engineering, in which porous, two-dimensional, or functional nanomaterials are incorporated within, beneath, or above the PA selective layer to regulate polymerization, create additional transport pathways, reinforce the network, or modify membrane interfaces. The following section therefore examines how filler-based design extends the molecular principles described above, while critically considering the associated challenges of polymer-filler compatibility, dispersion, interfacial defect formation, long-term stability, reproducibility, and scalable manufacture.

3. Nanostructuring and Filler Engineering in Nanofiltration Membranes

3.1 Thin-Film Nanocomposite and Mixed Matrix Membranes

In conventional polymeric membranes, separation behaviour is largely dictated by intrinsic polymer properties, such as chain packing, free-volume distribution, and hydrophilicity. However, the integration of functional nanofillers, including metal organic frameworks (MOFs), graphene derivatives, MXenes, zeolites, covalent organic frameworks (COFs), and other two-dimensional nanomaterials to form the so-called thin film nanocomposite (TFC) membranes and mixed matrix membranes (MMMs) introduces a complex interfacial region that fundamentally alters transport behaviour, structural stability, and long-term membrane performance. The scheme pictorially demonstrating the hierarchical evolution of the TFC and MMMs is presented in Figure 2. The interfacial domain between polymer and filler acts as a critical transition zone where molecular interactions, stress distribution, and transport pathways converge to determine the overall separation characteristics [41].

From a structure–performance perspective, the polymer–filler interface cannot be regarded simply as a passive boundary. Rather, it represents a dynamic physicochemical region whose structural organization governs permeability–selectivity trade–offs, fouling resistance, mechanical durability, and operational stability under realistic filtration conditions as shown in Figure 2. Understanding the physics of this interface, therefore, constitutes a central challenge in the rational design of advanced NF membranes. Recent advances in nanoscale characterization and molecular modelling have revealed that subtle variations in interfacial compatibility, interphase morphology, and defect formation mechanisms can lead to significant changes in membrane performance. Consequently, the design of high-performance MMMs requires careful control of interfacial interactions to maximize beneficial transport pathways while minimizing structural defects [42].

3.2 Interfacial Compatibility and Interphase Engineering

Interfacial compatibility between polymer matrices and nanofillers plays a decisive role in determining the structural integrity and separation performance of MMMs. Incompatible interfaces can lead to weak adhesion, void formation, and filler aggregation, all of which compromise membrane selectivity and mechanical stability. Conversely, strong polymer–filler interactions promote uniform filler dispersion and facilitate the formation of a well-defined interphase that contributes positively to mass transport regulation [43]. At the molecular level, compatibility is governed by several factors including surface chemistry of the filler, polymer chain mobility, and intermolecular forces such as hydrogen bonding, π–π interactions, electrostatic attraction, and van der Waals forces. Hydrophilic nanofillers incorporated into hydrophobic polymer matrices often exhibit poor dispersion due to unfavourable thermodynamic interactions, resulting in phase separation. To overcome these challenges, surface functionalization strategies have been widely employed to tailor filler surfaces with compatible chemical groups. Functional groups such as

hydroxyl, carboxyl, amine, and sulfonic moieties can enhance interfacial adhesion through hydrogen bonding or covalent interactions with polymer chains [44, 45].

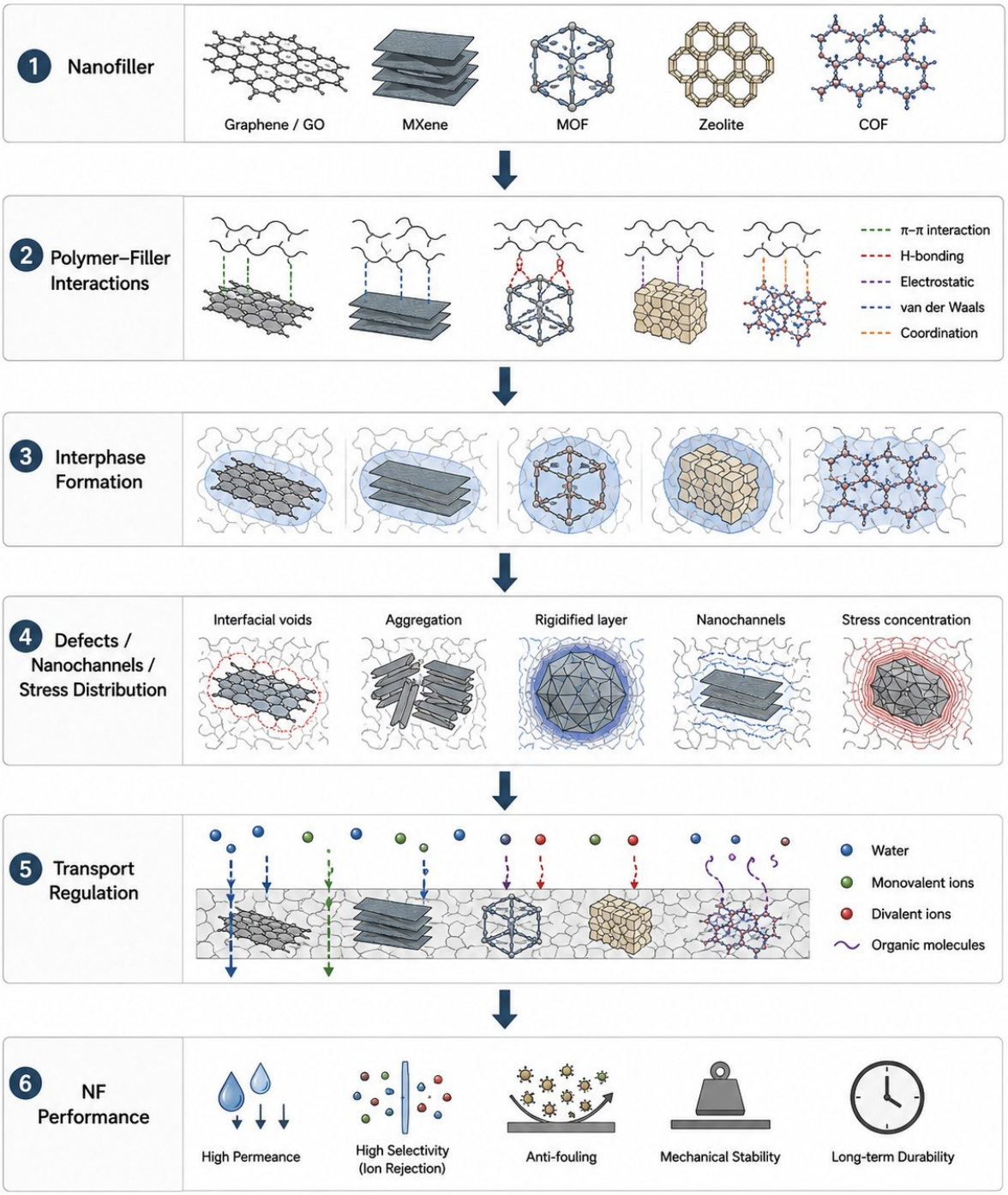

Figure 2. Schematic illustration of the hierarchical evolution of thin-film nanocomposite (TFC) and mixed matrix NF membranes, demonstrating the progression from nanofiller incorporation to system-level membrane performance.

While strong polymer-filler interactions are generally regarded as favourable for suppressing interfacial voids and enhancing dispersion, the strength of this interaction must be carefully balanced rather than simply maximized. Excessively strong

interfacial bonding can immobilize polymer chains near the filler surface, reducing local free volume and consequently restricting water permeability, a phenomenon reflected in the "rigidified polymer layer" defect mechanism discussed in next section. This indicates that an ideal interphase must provide sufficient adhesion to prevent defect formation while retaining adequate polymer chain mobility to sustain efficient molecular transport. For instance, moderate-density surface functionalization, such as partial hydroxylation or controlled grafting density, has been shown to preserve interfacial adhesion while avoiding excessive chain rigidification, thereby maintaining permeability without compromising selectivity. Similarly, optimizing filler loading below the threshold at which interfacial rigidification becomes dominant allows researchers to balance mechanical reinforcement with transport efficiency. These examples highlight those interfacial engineering strategies must be tailored not only to maximize adhesion strength but to optimize the balance between structural stability and transport performance.

In addition to chemical functionalization, the geometry and dimensionality of nanofillers strongly influence compatibility. Two dimensional nanomaterials such as graphene oxide and MXenes provide large surface areas for interaction with polymer chains, enabling the formation of extended interfacial regions. These interphases can significantly modify the local polymer packing structure, often leading to increased free volume or altered chain orientation. Such structural rearrangements may enhance water permeability while maintaining ion rejection, particularly in NF membranes designed for selective solute separation. Thermodynamic models and molecular simulations increasingly play an important role in predicting compatibility within MMM systems. Parameters such as solubility parameters, interfacial energy, and cohesive energy density are commonly used to estimate the likelihood of favorable interactions. By integrating these predictive approaches with experimental synthesis, researchers are now able to rationally design polymer–filler combinations that maximize interfacial stability and minimize aggregation [46].

3.3 Defect Formation Mechanisms in Mixed Matrix Membranes

Defect formation at the polymer–filler interface remains one of the most critical challenges in the development of high performance MMMs. These defects typically originate from insufficient interfacial adhesion, thermodynamic incompatibility between polymer chains and nanofillers, or structural heterogeneities introduced during membrane fabrication. Table 1 highlights the mechanism and impacts or effects of common interfacial defects on the MMMs' performance. Depending on the nature of the polymer filler interaction, these distinct defect morphologies in Table 1 may arise, including interfacial voids, filler aggregation, rigidified polymer layers, and polymer chain penetration into filler pores. Among these, interfacial voids represent the most detrimental defect type, as they create non selective transport pathways that bypass the selective polymer matrix and significantly reduce membrane rejection performance [47, 48]

Table 1. Common Interfacial Defects in MMMs and Their Mechanisms and Effects on Membrane Performance

Defect Type	Mechanism	Effect
Interfacial voids	Poor adhesion between polymer and filler	Non selective transport
Filler aggregation	Nanoparticle clustering	Heterogeneous microstructure
Rigidified polymer layer	Strong polymer–filler interaction immobilizes chains	Reduced permeability
Polymer chain penetration into filler pores	Polymer blocks porous filler	Loss of molecular sieving
Microcracks	Stress mismatch during drying or operation	Mechanical instability

In addition to chemical incompatibility, processing conditions during membrane fabrication also play a significant role in defect formation. Rapid solvent–nonsolvent exchange during phase inversion may induce filler migration and aggregation, leading to heterogeneous filler distribution across the membrane structure. Furthermore, differences in mechanical properties and thermal expansion coefficients between rigid nanofillers and flexible polymer matrices may generate localized stress concentrations during membrane drying or operation, resulting in microcrack formation. These defects disrupt the designed transport pathways and often lead to a deterioration of the permeability–selectivity balance that defines membrane separation efficiency [49].

To mitigate such interfacial defects, recent research has focused on interface engineering strategies including nanofiller surface functionalization, polymer grafting, and in situ growth of fillers within the polymer matrix. These approaches enhance polymer

filler compatibility and promote the formation of a stable interphase region that suppresses void formation while maintaining controlled molecular transport pathways [50].

3.4 Stress Concentration and Mechanical Stability

The incorporation of rigid nanofillers into polymer matrices inevitably alters the mechanical behaviour of MMMs. While nanofillers can enhance membrane stiffness and resistance to compaction, they may also introduce localized stress concentrations at the polymer–filler interface. These stress concentrations arise due to differences in elastic modulus between the filler and polymer phases, particularly when highly rigid materials such as inorganic nanoparticles or two dimensional nanosheets are embedded within relatively flexible polymer matrices. Under operational conditions typical of NF systems, such as elevated pressures, shear forces, and cyclic loading, these stress concentration zones can serve as initiation points for mechanical failure. Microcracks originating at the interface may propagate through the polymer matrix, leading to structural degradation and loss of membrane integrity over time. Therefore, understanding the mechanics of interfacial stress distribution is essential for designing mechanically robust membranes [51, 52].

Recent advances in nanomechanical characterization techniques, including atomic force microscopy (AFM) nanoindentation and nano dynamic mechanical analysis, have enabled detailed investigation of interfacial mechanical properties at the nanoscale. These techniques reveal that the interphase region surrounding nanofillers often exhibits mechanical properties distinct from both the bulk polymer and the filler itself. In many cases, polymer chains near the filler surface become immobilized, forming a rigid interfacial layer that contributes to enhanced mechanical reinforcement. As noted in Section 3.2, this reinforcement must be balanced against the associated risk of reduced permeability due to interfacial chain rigidification. The design of mechanically stable MMMs therefore requires careful optimization of filler loading, particle size, and dispersion state. Excessive filler content may lead to particle–particle interactions that amplify stress concentration effects, whereas moderate filler incorporation with strong interfacial bonding can effectively distribute mechanical stresses throughout the membrane matrix. Surface functionalization and polymer grafting strategies are particularly beneficial in this context, as they promote gradual stress transfer across the interface rather than abrupt mechanical discontinuities.

3.5 Interfacial Transport Pathways and Nanochannel Engineering

The polymer–filler interface not only influences structural integrity but also plays a crucial role in regulating molecular transport within NF membranes. In many MMM systems, the interfacial region forms preferential transport pathways that differ significantly from those in the bulk polymer matrix. These pathways pictorially illustrated in Figure 3 arise due to modifications in polymer chain packing, interfacial free volume, and the presence of nanoscale channels associated with the filler structure [53].

For example, two dimensional nanomaterials such as graphene oxide and MXenes can create layered nanochannels that facilitate rapid water transport while restricting the passage of larger solutes or multivalent ions. Similarly, porous fillers such as MOFs and zeolites provide intrinsic molecular sieving properties that enhance selectivity. However, the effectiveness of these transport pathways depends strongly on the continuity and connectivity between the filler pores and the surrounding polymer matrix [54], [55]. The interfacial region may also influence transport through the formation of an “interphase layer,” where polymer chain mobility and free volume differ from those in the bulk material. This modified region can act either as a barrier or as an accelerator for molecular diffusion, depending on the nature of polymer–filler interactions. For instance, strong interfacial interactions that immobilize polymer chains may reduce free volume and hinder transport, whereas weak interactions may create additional free volume that enhances permeability.

Advanced modelling approaches, including molecular dynamics simulations and continuum transport models, have provided valuable insights into the role of interfacial regions in determining membrane performance. These studies suggest that optimizing the interfacial structure can enable membranes to overcome traditional permeability selectivity trade-offs, a key objective in the development of next generation NF systems [56].

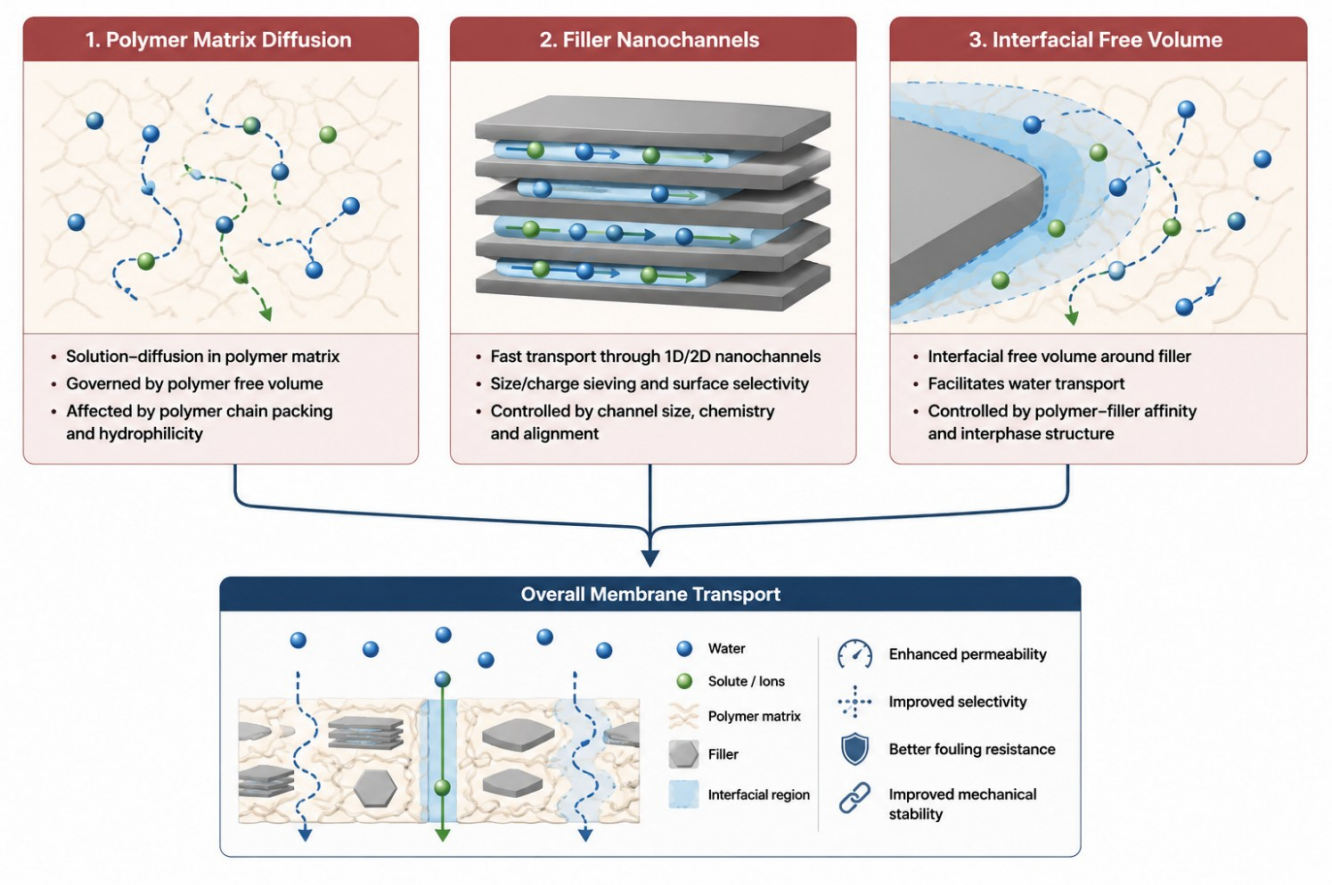

Figure 3. Schematic representation of water and solute transport pathways in mixed matrix membranes (MMMs), illustrating the three primary transport mechanisms: (1) diffusion through the polymer matrix, (2) fast transport through filler nanochannels, and (3) interfacial free volume around the filler. The combined effects lead to enhanced permeability, improved selectivity, better fouling resistance, and improved mechanical stability.

3.6 Characterization Challenges and Multiscale Analysis

Despite significant progress in MMM design, the direct characterization of polymer–filler interfaces remain a formidable challenge due to the nanoscale dimensions and complex morphology of the interfacial region. Conventional characterization techniques often lack the spatial resolution necessary to probe interfacial phenomena or to distinguish between the polymer matrix, filler particles, and interphase layers [46, 57].

Electron microscopy techniques such as transmission electron microscopy (TEM) and scanning electron microscopy (SEM) provide valuable information regarding filler dispersion and membrane morphology; however, they often fail to capture subtle interfacial interactions at the molecular level. Spectroscopic methods including Fourier transform infrared spectroscopy (FTIR), Raman spectroscopy, and X-ray photoelectron spectroscopy (XPS) are frequently employed to identify chemical bonding and functional group interactions between polymers and fillers. Nevertheless, these techniques typically provide averaged information rather than spatially resolved insights [58, 59]. Recent developments in advanced characterization techniques have begun to address these limitations. Techniques such as scanning transmission electron microscopy (STEM), electron energy loss spectroscopy (EELS), and atomic force microscopy (AFM) based methods enable higher resolution analysis of interfacial structures. Computational modelling also plays an increasingly important role in bridging experimental gaps. Multiscale simulations combining molecular dynamics with continuum transport models provide insights into interfacial behaviour that

cannot be easily obtained experimentally. By integrating advanced characterization with theoretical modelling, researchers are gradually developing a more comprehensive understanding of polymer–filler interface physics.

Although nanomaterials and advanced fabrication strategies can introduce new transport pathways, their ultimate contribution to membrane performance depends strongly on the resulting nanoscale morphology and interfacial structure. Understanding the relationship between structural evolution and separation behaviour is therefore essential for distinguishing genuine performance improvements from experimentally observed but poorly understood enhancements.

4. Morphology-Performance Correlations in Nanofiltration Membranes

4.1 Surface Roughness and Permeability Trade-Offs

Membrane surface morphology is a critical structural parameter governing permeability, fouling behaviour, and selective transport in NF membranes. Surface roughness, typically characterized using AFM, directly influences mass transfer across the membrane interface and modulates the interaction between the membrane surface and foulants during filtration processes[60], [61]. NF membranes fabricated via interfacial polymerization generally exhibit ridge-and-valley morphologies, which generate heterogeneous transport pathways across the membrane surface [60]. Surface roughness exerts a dual influence on membrane performance. Moderate roughness can enhance water permeance by increasing the effective interfacial area available for transport. Conversely, excessive roughness promotes the formation of microscopic valleys that function as deposition sites for colloids, organic matter, and biological species, accelerating fouling and flux decline [60, 61] as shown in Figure 4.

A comparative analysis across different membrane systems illustrates this complexity (Table 2). In polyamide NF membranes, moderate roughness increases (19–25 nm) have been shown to significantly enhance water permeance due to surface area expansion [62] as illustrated in Figure 4. However, such roughness effects are highly system-dependent and cannot be directly compared across different membrane chemistries and operating conditions alone. The extent to which increased roughness improves permeance or influences fouling behaviour is tightly coupled with surface chemistry, underlying pore structure, and foulant properties rather than the roughness magnitude in isolation. In contrast, smoothening modified polyether sulfone (PES) NF membranes enhanced long-term stability, hydrophilicity, and fouling resistance, despite a reduction in intrinsic roughness.

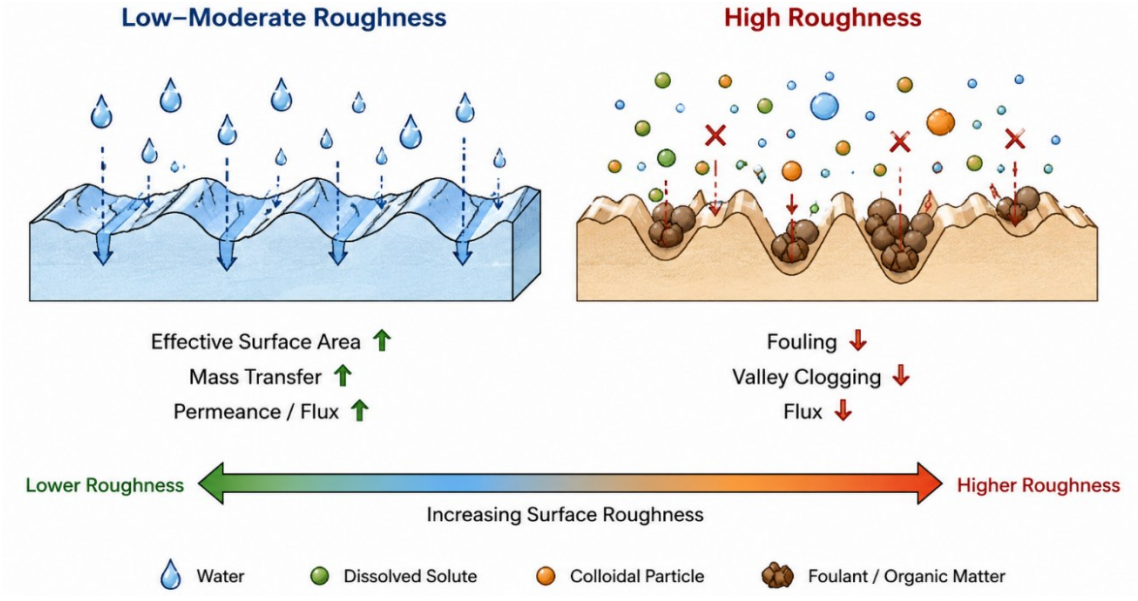

Figure 4. Schematic illustrating permeance enhancement and fouling mechanisms as a function of membrane surface roughness.

Table 2. Summary of the effect of membrane surface roughness on permeability and flux across different membrane types and operating regimes.

Study	Membrane Type	Roughness (Ra)	Permeability / Flux	Operating Regime	Observed Trend	Key Mechanism
[61]	PES NF	45.8 nm → 1.3 nm	Higher stability for smoother membranes	Pressure-driven (NF)	Roughness decreased after modification	Reduced fouling & improved hydrophilicity
[62]	Polyamide NF	19–25 nm	5.8 → 10.6 LMH/bar	Pressure-driven (NF)	Increased flux with moderate roughness	Larger effective surface area
[63]	PVDF MF	rough vs. smooth	Smooth membrane, higher flux	Pressure-driven (MF)	Rough surfaces cause valley clogging	Particle deposition
[64]	UF/MF membranes	63–247 nm	Rough membranes have a higher stabilized flux.	Gravity-driven, biofilm-assisted (GDM)	Biofilm-assisted permeability	Bioactive fouling layer structure

Studies on PVDF microfiltration membranes similarly indicate that smoother surfaces exhibit higher and more stable flux, as rougher membranes suffer from enhanced particle deposition and valley clogging [63]. However, in a gravity-driven UF/MF membrane system, higher surface roughness has been associated with improved stabilized flux due to the formation of a structured biofilm layer that facilitates water transport [64]

The influence of surface roughness on performance can be rationalized through two competing mechanisms that explain the relationship between roughness and permeability, as illustrated in Figure 4. Firstly, surface area enhancement occurs when the membrane-solution interfacial area is increased in roughness, reducing localized transport resistance and improving permeance. This mechanism has been experimentally validated in modified NF membranes displaying modest roughness amplification [60], [61]. In contrast, the fouling accumulation mechanism dominates at higher roughness amplitudes. Microscopic valleys formed on rough membrane surfaces preferentially trap suspended particles and macromolecules, intensifying pore blockage and promoting irreversible fouling [60]. The accumulation of foulants within these recessed regions reduces effective pore accessibility and accelerates permeate flux decline during prolonged filtration. The net performance outcome, therefore, depends on the balance between roughness-induced permeability enhancement and fouling resistance influenced by surface chemistry, hydrophilicity, pore structure, and foulant characteristics.

4.2 Pore Size Distribution, Selective Layer Thickness, and Their Interdependence

NF separation performance is governed jointly by pore size distribution (PSD) and selective layer thickness, two morphological parameters that arise from a common fabrication mechanism and are therefore considered together rather than independently.

Separation in NF membranes is predominantly governed by size exclusion, whereby solutes smaller than the effective pore size permeate while larger species are rejected. NF membranes typically exhibit pores on the order of 1-2 nm, with molecular weight cut-off (MWCO) values between 200-1000 Da, enabling rejection of multivalent ions and larger organic molecules while permitting water and smaller solutes to pass. A narrow, uniform PSD is essential for high rejection, since broad distributions permit preferential flow through oversized pores; PSD characterization is nonetheless complicated by the fact that pore dimensions measured under dry conditions can differ substantially from effective pore sizes under hydrated operation, owing to polymer swelling and structural rearrangement [64].

Selective layer thickness governs hydraulic resistance and therefore controls both permeability and rejection [68]. Permeability in porous membranes follows the Hagen–Poiseuille relationship, in which permeate flux scales inversely with transport path length. Reducing selective layer thickness accordingly enhances permeance; thin-film nanocomposite NF membranes with active layers of 80-120 nm typically balance permeability against selectivity, whereas excessive thinning induces structural defects that compromise rejection [65].

These two parameters, together with surface roughness (Section 4.1), originate from the same amine-diffusion and interfacial-reaction kinetics that govern interfacial polymerization and cannot be tuned independently. Any strategy that alters monomer diffusion, whether through interlayer incorporation, additive-regulated diffusion, or changes in reaction time and concentration, simultaneously reshapes the thickness, roughness, and pore architecture of the resulting polyamide layer. Regulating piperazine diffusion with a charged interlayer, for instance, concurrently reduces selective-layer thickness, increases surface roughness, and narrows the pore-size distribution. Likewise, varying interlayer composition and deposition time simultaneously alters pore size, porosity, surface roughness, and selective-layer thickness, with all parameters shifting together as diffusion conditions change. Roughness, PSD, and thickness are therefore best understood as co-varying outputs of a single fabrication mechanism rather than as independently addressable design targets.

This coupling constrains morphology-driven optimization in practice. Thinning the selective layer to reduce transport resistance frequently increases surface roughness and broadens the pore-size distribution, since thinner, less-crosslinked films are more prone to localized defects and non-uniform growth during polymerization [65], the resulting permeance gain can therefore be partially offset by reduced selectivity or accelerated fouling, as rougher, more heterogeneous surfaces provide additional deposition sites for foulants (Section 4.1). Conversely, narrowing the pore-size distribution to improve rejection precision typically requires slower, more tightly controlled polymerization, which increases layer thickness and can suppress permeance [64]. Because the fabrication conditions that improve one parameter tend to degrade another, roughness, PSD, and thickness cannot be optimized sequentially or in isolation.

Morphology optimization for NF membranes is therefore inherently a multi-objective problem. Rather than tuning roughness, pore size distribution, and thickness independently, membrane design should target fabrication conditions, such as interlayer chemistry, monomer concentration, and reaction time, that shift the coupled parameter set toward a favourable joint operating point, evaluated through combined characterization (AFM, porosimetry, and cross-sectional TEM/ellipsometry) rather than any single morphological descriptor.

The complexity of multiscale structural features, ranging from molecular-level interactions to macroscopic membrane morphology, makes experimental optimization alone insufficient for establishing predictive design principles. Consequently, computational modelling and simulation approaches have become increasingly important for quantitatively linking membrane structure with transport mechanisms.

5. Advanced Modelling and Predictive Frameworks

The advancement of NF and MMMs for water treatment increasingly depends on predictive modelling frameworks capable of resolving transport phenomena across multiple length scales shown in Figure 5. In water purification systems, separation performance is governed by coupled mechanisms including steric hindrance, electrostatic interactions, dielectric exclusion, adsorption, and concentration polarization. These processes occur simultaneously across nanoscale pores, mesoscale membrane architectures, and macroscale filtration modules, making empirical optimization insufficient for rational membrane design.

Recent developments highlight that transport behaviour in NF membranes deviates from classical continuum assumptions due to nanoscale confinement and interfacial effects. These deviations become more pronounced in MMMs, where heterogeneous interfaces between polymer and filler materials introduce additional resistance pathways and preferential transport channels. Consequently, predictive frameworks integrating molecular simulations (e.g., molecular dynamics (MD) and quantum mechanics like DFT simulation), pore network modelling, and continuum transport models have emerged as essential tools for designing high-performance membranes for water treatment applications [66-69] as illustrated in Figure 5.

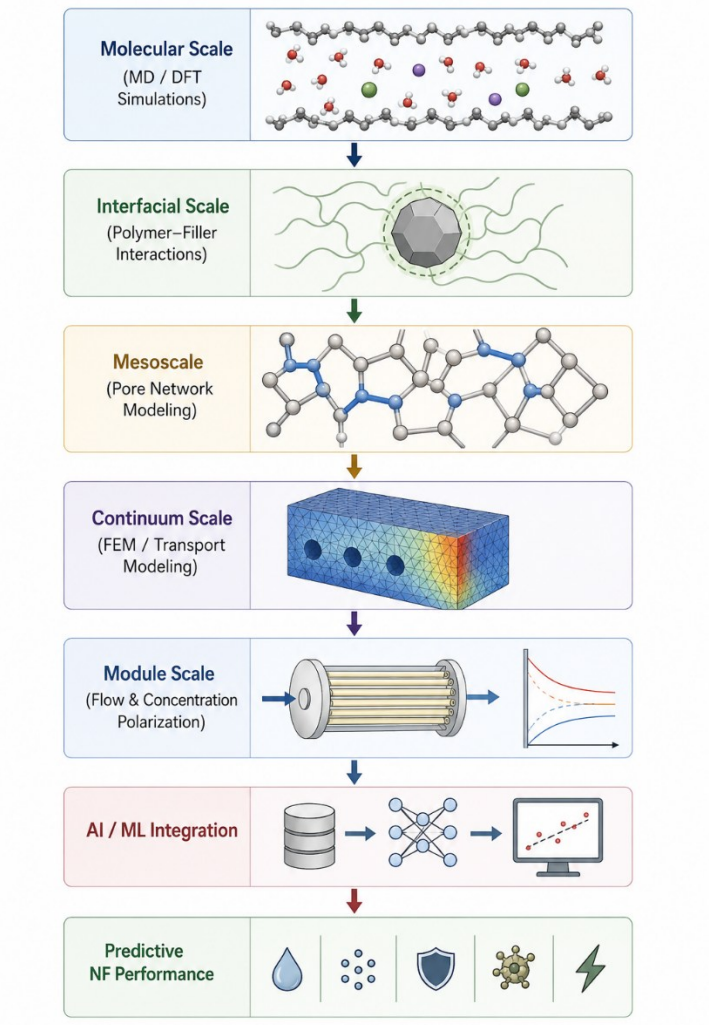

Figure 5. Schematic illustration of the multiscale predictive modelling framework for NF and MMMs.

5.1 Molecular Simulations

Molecular simulations provide mechanistic insights into nanoscale transport phenomena that govern separation performance in NF and MMMs. In water treatment applications, molecular dynamics (MD) simulations have demonstrated that solvent transport within nanopores deviates significantly from classical hydrodynamic behaviour due to molecular confinement and surface interactions. Water molecules form structured layers near pore walls, reducing effective diffusivity and generating additional transport resistance. These findings challenge conventional solution–diffusion models and highlight the importance of surface chemistry and pore architecture in controlling membrane performance [70].

In MMMs for water purification, molecular simulations are particularly useful for analyzing polymer–filler interfacial effects. Transport resistance often originates from polymer rigidification near filler surfaces, which reduces free volume and slows diffusion. Conversely, interfacial void formation can increase permeability but may compromise selectivity. These competing mechanisms explain the frequently observed permeability–selectivity trade-off in MMMs used for desalination and wastewater treatment.

Additionally, molecular simulations have been employed to investigate adsorption-driven separation mechanisms for contaminants such as heavy metals, dyes, and organic micropollutants. Nanoporous fillers such as metal–organic frameworks

(MOFs), graphene oxide, and silica nanoparticles exhibit selective adsorption behaviour that enhances rejection performance. However, simulation studies reveal that adsorption enhancement is often limited by interfacial resistance between filler and polymer phases, highlighting the importance of interfacial engineering in MMM design [71].

Despite their mechanistic advantages, molecular simulations remain constrained by time scale and computational cost limitations. Transport processes in water treatment membranes occur over milliseconds to seconds, whereas molecular simulations typically operate at nanosecond time scales. Additionally, realistic MMM structures with heterogeneous filler distributions remain computationally challenging to model. To address these limitations, coarse-grained simulations and machine learning-assisted molecular modelling approaches are increasingly employed to extend simulation scales and improve predictive accuracy.

5.2 Pore network Modelling

Pore network modelling (PNM) provides a mesoscale framework for analyzing heterogeneous membrane structures commonly observed in NF and MMMs. In water treatment applications, membrane performance depends strongly on pore size distribution, tortuosity, surface charge, and connectivity. Traditional uniform pore models fail to capture these complexities, leading to inaccurate prediction of rejection performance and permeability. The Donnan–Steric Pore Model with Dielectric Exclusion (DSPM-DE) remains one of the most widely used mechanistic frameworks for NF modelling. This model incorporates steric exclusion, electrostatic interactions, and dielectric effects, enabling prediction of ion rejection behaviour in water treatment systems. However, DSPM-DE assumes uniform pore geometry and neglects structural heterogeneity, limiting its predictive accuracy for advanced NF membranes and MMMs [72].

Pore network modelling addresses these limitations by representing membranes as interconnected pore networks with varying pore sizes and surface properties. This approach allows evaluation of transport pathways and bottlenecks, particularly relevant for MMMs where filler dispersion significantly affects performance. Well-dispersed fillers create preferential transport pathways, while agglomeration introduces dead zones that reduce membrane efficiency as illustrated in Figure 5. Recent advances in pore network modelling incorporate electrostatic interactions, adsorption effects, and concentration polarization, which are critical for water purification applications. Additionally, pore networks reconstructed from imaging techniques such as electron microscopy and X-ray tomography enable realistic representation of membrane structures. These developments improve predictive accuracy and facilitate rational membrane design.

5.3 Finite Element Transport Modelling

Finite element modelling (FEM) shown in Figure 5 provides a continuum-scale framework for analyzing coupled transport phenomena in NF and MMMs. Different modelling approaches operate at distinct length scales, each offering unique advantages and limitations. In water treatment applications, separation performance depends strongly on concentration polarization, pressure distribution, and flow dynamics within membrane modules. Finite element models enable simultaneous solution of governing equations including Navier–Stokes equations, convection–diffusion equations, and electrostatic transport equations.

Concentration polarization significantly reduces membrane performance by increasing solute concentration near the membrane surface. Finite element simulations have demonstrated that concentration polarization leads to reduced flux and decreased rejection efficiency in NF systems. These effects become more pronounced in high-salinity wastewater treatment applications and desalination processes [73].

Finite element modelling (FEM) is also useful for analyzing MMMs by explicitly representing filler particles within polymer matrices. These simulations reveal that filler geometry, loading, and interfacial properties strongly influence transport behaviour. For example, large filler particles may create transport resistance zones, while nanoscale fillers enhance permeability by creating additional transport pathways. Furthermore, finite element modelling enables simulation of module-level performance, including crossflow velocity, feed composition, and operating pressure. These factors significantly influence membrane performance but

are often neglected in smaller-scale models. Recent Multiphysics FEM approaches also incorporate fouling layer formation, membrane deformation, and temperature effects, providing insight into long-term membrane performance.

5.4 Multiscale Modelling Frameworks

Multiscale modelling frameworks aim to integrate molecular simulations, pore network modelling, and finite element transport modelling into a unified predictive framework. In water treatment membranes, separation performance emerges from nanoscale interactions that propagate through mesoscale pore networks to macroscale filtration modules, illustrated in Figure 5. Molecular simulations provide nanoscale parameters such as diffusion coefficients, adsorption energies, and interfacial resistance. These parameters are incorporated into pore network models, which capture structural heterogeneity and transport pathways. The resulting outputs are then used in finite element models to predict module-level performance.

Recent multiscale modelling studies demonstrate that dynamic pore structures and nanoscale heterogeneity strongly influence NF performance. These findings highlight the importance of integrating multiple modelling approaches for accurate prediction of membrane behaviour. Machine learning and data-driven approaches are emerging as powerful tools for linking nanoscale structure to macroscale performance. By integrating simulation data and experimental measurements, machine learning models can identify structure–performance relationships and accelerate membrane design. Future research should focus on developing hybrid modelling frameworks combining physics-based modelling and data-driven approaches. Such frameworks will enable predictive design of NF and MMMs for water treatment applications, reducing experimental workload and accelerating commercialization.

While molecular simulations and mechanistic models provide fundamental insights into structure-transport relationships, their application is often limited by computational cost and the complexity of high-dimensional design spaces. Data-driven approaches and artificial intelligence provide complementary strategies for extracting hidden patterns and accelerating the discovery of optimized membrane structures.

6. Artificial Intelligence and Data-Driven Membrane Design

NF membranes are often characterized by the pore sizes range 1–2 nm and molecular weight cut-offs of 200–1000 Da, occupy a paramount position in diverse practical applications like water treatment, pharmaceutical separations, and critical mineral recovery [74]. Compared to reverse osmosis, NF operates at lower transmembrane pressures while still eliminating divalent ions and natural organic matter effectively attributes that emphasize its role in next-generation desalination and wastewater valorization [75]. Conventionally, balanced NF design has been restrained by vast, interacting parameters such as polymer type, solvent system, additive concentration, and phase inversion kinetics that conventional experimental approaches handle inefficiently [76]. AI addresses this directly by extracting latent structure–property relationships from large, heterogeneous datasets, enabling systematic navigation of a design landscape that would otherwise take decades to explore manually [77, 78].

The quality and scope of data fundamentally determine machine-learning model capability. Recent studies have demonstrated the potential of ML for polymeric membrane design while highlighting challenges associated with data collection, preparation, limited observations, and data augmentation [79,80]. ML frameworks have also been developed specifically for nanofiltration and reverse-osmosis membrane optimization and pollutant removal [81]. Transfer-learning and active-learning strategies can further alleviate data scarcity, although evidence should be cited from studies directly demonstrating these approaches [82]. Meanwhile, automated high-throughput membrane fabrication and characterization platforms are emerging as a foundation for data-driven and potentially closed-loop membrane optimization [83,84].

6.1 Machine Learning and Deep Learning for Performance Prediction

Supervised NF performance models such as random forests, gradient boosted trees, and support vector regression represent the most widely used AI paradigm for performance forecasting. XGBoost trained on 2,400 data points has been shown to predict

sodium chloride (NaCl) and magnesium sulphate ($MgSO_4$) rejection with $R^2 = 0.96$ and MAE below 3%, with SHAP analysis confirming that polymer crosslinking density and surface zeta potential are the dominant interpreters [85, 86]. For multi-ion systems, multitask learning has been applied to simultaneously predict rejection coefficients for five ions with R^2 above 0.93 in each case, enforcing physical bounds through custom loss functions [87].

Deep learning models (DLM) have proven valuable as far as time-dependent phenomena are concerned. LSTM networks proficient on 18 months of pilot data with predicted flux decline of 72 hours in advance with 95% accuracy, enabling proactive chemical cleaning that automatically cut reagent use by 31%. CNN (Convolutional Neural Network) architectures particularly ResNet-50 fine-tuned on 6,000 labelled SEM cross-sections classify fouling severity with 97.2% accuracy, reducing reliance on expert interpretation [88]. Transformer-based models have also been adapted to sequence fabrication steps as demonstration inputs, predicting final membrane physical structure from synthesis protocols with replication-level accuracy [89].

Graph neural networks encode molecular structures as graphs, allowing direct learning from chemical topology without hand-crafted descriptors [90]. A junction tree variational autoencoder was used to generate novel polyamide monomers targeting specific permeance and rejection values; two of five synthesized candidates showed Pareto-superior performance compared to commercial membranes [91]. Conditional GANs (Generative Adversarial Networks) were employed for inverse design of polyimide NF membranes, computationally screening over ten million candidate structures in 48 hours, a breadth estimated at four decades of conventional experimentation [92]. Graph-based approaches have additionally been applied to predict chemical stability and solvent resistance, encoding pH and interaction parameters alongside structural features for a complete materials screening workflow [87].

Data driven models have risk in physically inconsistent predictions, particularly when extrapolating beyond training distributions. Physics-informed neural networks (PINNs) resolve this drawback by embedding governing equations the solution-diffusion model, Nernst-Planck transport, and Hagen-Poiseuille pore flow as constraints in the loss function [93]. PINN embedding the extended Nernst-Planck equation has been shown to match finite-element simulations in accuracy while reducing computation time manyfold, enabling real-time transport modelling within digital twin frameworks [94]. Hierarchical hybrid approaches couple with the DFT, molecular dynamics, and gradient-boosted proxies further allow macroscopic performance to be predicted from polymer chain architecture alone, with free energy RMSE below 1.2 kJ/mol [95].

6.2 Multi-Objective Optimization and Autonomous Membrane Discovery

Directing these two features in the filtration membranes permeability, selectivity Pareto frontier requires optimization algorithms that operate across the multiple competing objectives simultaneously. NSGA-III coupled with an ML substitute was used to optimize five fabrication parameters for polyethersulfone (PES) NF membranes, identifying compositions that exceeded the traditional trade-off upper bound while requiring 87% fewer experiments than full factorial design [96]. A self-driving laboratory has also been introduced, in which a Bayesian optimization agent directed robotic synthesis, characterization, and evaluation in a closed loop over 14 days, discovering ternary solvent formulations that improved selectivity by 38% without human intervention [97]. Reinforcement learning has complemented this direction: a PPO agent trained in a pilot NF system reduced specific energy consumption by 22% while maintaining regulatory permeate quality [98].

Large language models (LLM) introduce a distinct capability synthesizing knowledge from unstructured literature at scale. A fine-tuned LLM has been applied to extract structured performance data from 12,000 journal articles in 14 days, assembling a validated database three times larger than any manually curated equivalent, with 91% accuracy [99]. Beyond curation, LLM-assisted hypothesis development has proposed under explored material combinations including bio-inspired zwitterionic coatings modelled on cell membrane lipid bilayers that were subsequently validated experimentally, demonstrating the potential of LLMs as catalysts for cross-disciplinary discovery [100].

6.3 Digital Twins and Intelligent Membrane Systems

Digital twin frameworks, virtual replicas of membrane systems continuously updated with real-time sensor data, enable predictive maintenance, virtual process optimization, and operator training, thereby reducing downtime as well as chemical and material costs. [101]. A typical workflow for its deployment is presented in Figure 6.

Federated learning complements this by enabling model training across multiple data owners without centralizing proprietary datasets; a seven-utility federated pipeline demonstrated an 18% improvement in fouling prediction accuracy over any single-site model [102]. Looking forward, persistent challenges include model interpretability and dataset bias toward idealized laboratory conditions. Quantum-ML integration and FAIR data standardization represent key longer-term frontiers for the field [103, 104].

However, membrane performance cannot be evaluated solely based on initial permeability and selectivity. Structural features that enhance transport, including surface chemistry, charge distribution, and nanochannel characteristics, also strongly influence fouling behaviour and long-term stability. Therefore, understanding structure-dependent surface interactions is essential for developing practically viable NF membranes.

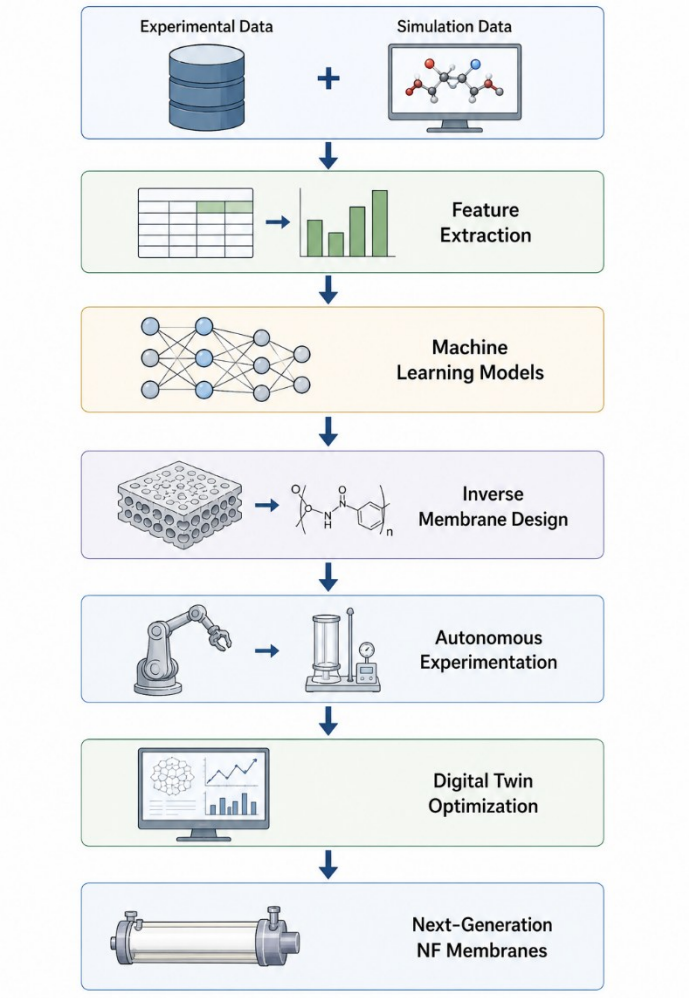

Figure 6. Schematic of a data-driven workflow integrating machine learning and digital twins for next-generation NF membrane design

7. Fouling Mechanisms and Surface Interactions

Membrane fouling remains one of the most critical challenges limiting the long-term performance, stability, and economic feasibility of NF and MMMs. Fouling refers to the accumulation of undesirable materials on membrane surfaces or within membrane pores, resulting in a decline in permeate flux, deterioration in selectivity, and increased operational costs due to cleaning and replacement requirements. In practical water treatment and industrial separation processes, fouling arises from complex interactions between membrane surfaces and various foulants present in feed streams, including organic macromolecules, microorganisms, and inorganic salts [105, 106]. In next-generation membranes, the relationship between membrane structure and fouling behaviour has become a central research focus. Surface chemistry, pore size distribution, surface charge, hydrophilicity, and roughness strongly influence foulant adsorption and deposition [107]. Nanostructured membranes incorporating functional nanomaterials such as graphene oxide (GO), metal–organic frameworks (MOFs), metal oxide nanoparticles, and other functional fillers offer new opportunities to tailor surface interactions and mitigate fouling [108]. Understanding the mechanisms governing fouling and the physicochemical interactions between membranes and foulants is therefore essential for designing high-performance NF and MMMs with improved antifouling properties. This section discusses the major fouling mechanisms in NF membranes, including organic fouling, inorganic scaling and biofouling, which is presented in Figure 7.

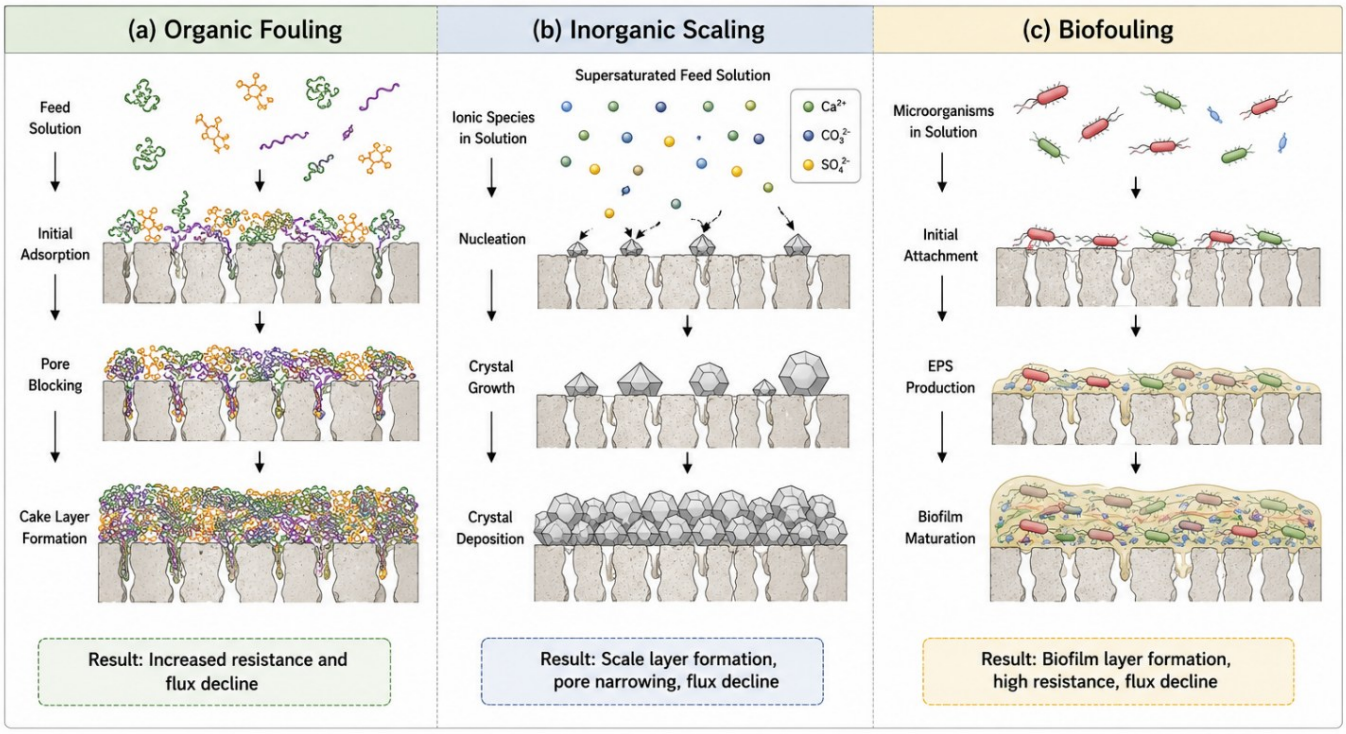

Figure 7. Schematic representation of the three major membrane fouling mechanisms: (a) organic fouling, (b) inorganic scaling, and (c) biofouling

In Figure 7, we presented different illustrations showcasing the different fouling mechanism in NF membranes. In addition, the hydration layer theory and emerging surface modification strategies are examined as key approaches for improving antifouling performance in next-generation membranes.

7.1 Organic Fouling

Organic fouling is one of the most prevalent forms of membrane fouling in NF processes, particularly in water purification and wastewater treatment applications. It occurs when dissolved organic compounds present in feed streams accumulate on the membrane surface or within pores, forming a fouling layer that restricts mass transport. Typical organic foulants include natural organic matter (NOM), proteins, polysaccharides, humic substances, and industrial organic contaminants [109]. The deposition of the species increases hydraulic resistance across the membrane, resulting in a significant decline in permeate flux and overall filtration performance. The progressive build-up of such organic matter on membrane surfaces has been reported to be a major contributor to irreversible fouling and long-term flux deterioration [110]. The fouling process is governed by several physicochemical interactions, including hydrophobic interactions, electrostatic attraction, hydrogen bonding, and van der Waals forces. Membrane surfaces with high hydrophobicity tend to adsorb organic molecules more readily due to strong hydrophobic interactions. For example, hydrophobic polymeric membranes such as polyethersulfone (PES) or polysulfone (PSF) often experience significant fouling when treating waters containing humic acids or proteins [111]. Surface charge also plays an important role in organic fouling behaviour. Electrostatic repulsion between negatively charged membrane surfaces and negatively charged organic molecules can reduce fouling propensity. The pore structure of the membrane further influences fouling behaviour, as smaller pores may become blocked by macromolecules, leading to pore constriction and flux decline. Increased crosslinking density in the selective layer reduces free-volume voids that would otherwise trap organic macromolecules, thereby lowering irreversible fouling but often at the cost of reduced permeance, illustrating the structure–fouling–performance trade-off central to next-generation membrane design

7.2 Inorganic Scaling

Inorganic scaling occurs when dissolved inorganic salts in feed solutions precipitate and accumulate on membrane surfaces or within membrane pores. The illustration is presented in Figure 7. Common scaling species include calcium carbonate ($CaCO_3$), calcium sulfate ($CaSO_4$), barium sulfate ($BaSO_4$), and silica. Scaling typically occurs when the concentration of these salts exceeds their solubility limits under operating conditions. The formation of scale deposits involves nucleation, crystal growth, and deposition processes. Membrane surfaces serve as nucleation sites where crystallization begins. Once crystals form, they grow and accumulate, eventually forming a dense layer that significantly reduces membrane permeability. Major flux decline in the membrane has been attributed to coupled inorganic–organic fouling, driven by salt precipitation, Ca^{2+}-natural organic matter complexation, and dense cake layer formation. They further highlighted that membrane surface roughness promoted nano colloid deposition and valley plugging, intensifying resistance to water permeation [112]. These findings illustrate that nanoscale surface roughness, rather than scaling chemistry alone, is often the dominant structural determinant of long-term flux decline in inorganically fouled membranes. Scaling is strongly influenced by membrane surface properties, operating conditions, and feed solution chemistry. Surface roughness and surface energy can affect nucleation behaviour, while local concentration polarization near the membrane surface can accelerate supersaturation and crystal formation.

7.3 Biofouling

Biofouling in Figure 7 refers to the accumulation and growth of microorganisms on membrane surfaces, resulting in the formation of biofilms. It is one of the most complex and persistent fouling mechanisms in membrane processes. Biofouling typically occurs through a multi-step process involving microbial attachment, growth, extracellular polymeric substance (EPS) production, and biofilm maturation. The initial stage of biofouling involves the adsorption of organic conditioning layers on the membrane surface. These layers provide nutrients and attachment sites for microorganisms. Once microbial cells attach to the surface, they begin to proliferate and secrete EPS, which consists of proteins, polysaccharides, lipids, and nucleic acids. The EPS matrix forms a protective biofilm that strongly adheres to the membrane surface and significantly increases permeance resistance. Biofouling can cause severe operational problems in NF systems, including flux decline, increased pressure requirements, and deterioration in membrane selectivity. In addition, biofilms may alter local chemical conditions at the membrane surface, potentially accelerating other fouling mechanisms such as inorganic scaling [113]. Incorporation of antimicrobial nanofillers (e.g., Ag, ZnO,

GO) alters surface charge and local reactive oxygen species generation, directly suppressing initial microbial attachment, the rate-limiting step in biofilm-driven performance decline.

7.4 Hydration Layer Theory

The hydration layer theory pictorially represented in Figure 8 has emerged as an important framework for understanding antifouling membrane surfaces. According to this theory, highly hydrophilic membrane surfaces can bind water molecules strongly through hydrogen bonding or electrostatic interactions, forming a tightly bound hydration layer. This layer acts as a physical and energetic barrier that prevents foulants from directly contacting the membrane surface.

Hydration layers are particularly effective at resisting protein adsorption, organic fouling, and microbial attachment. When foulant molecules approach the membrane surface, they must displace the bound water molecules within the hydration layer. Because this process requires significant energy, foulant adsorption becomes thermodynamically unfavorable. Zwitterionic polymers are among the most effective materials for generating stable hydration layers. These materials contain both positive and negative charged functional groups, which strongly interact with water molecules and create highly hydrated surfaces. Membranes modified with zwitterionic coatings have demonstrated exceptional antifouling properties in various water treatment applications. This confirms that surface hydrophilicity is not merely a passive membrane characteristic but an actively tuneable structural parameter that directly governs fouling resistance and long-term flux stability.

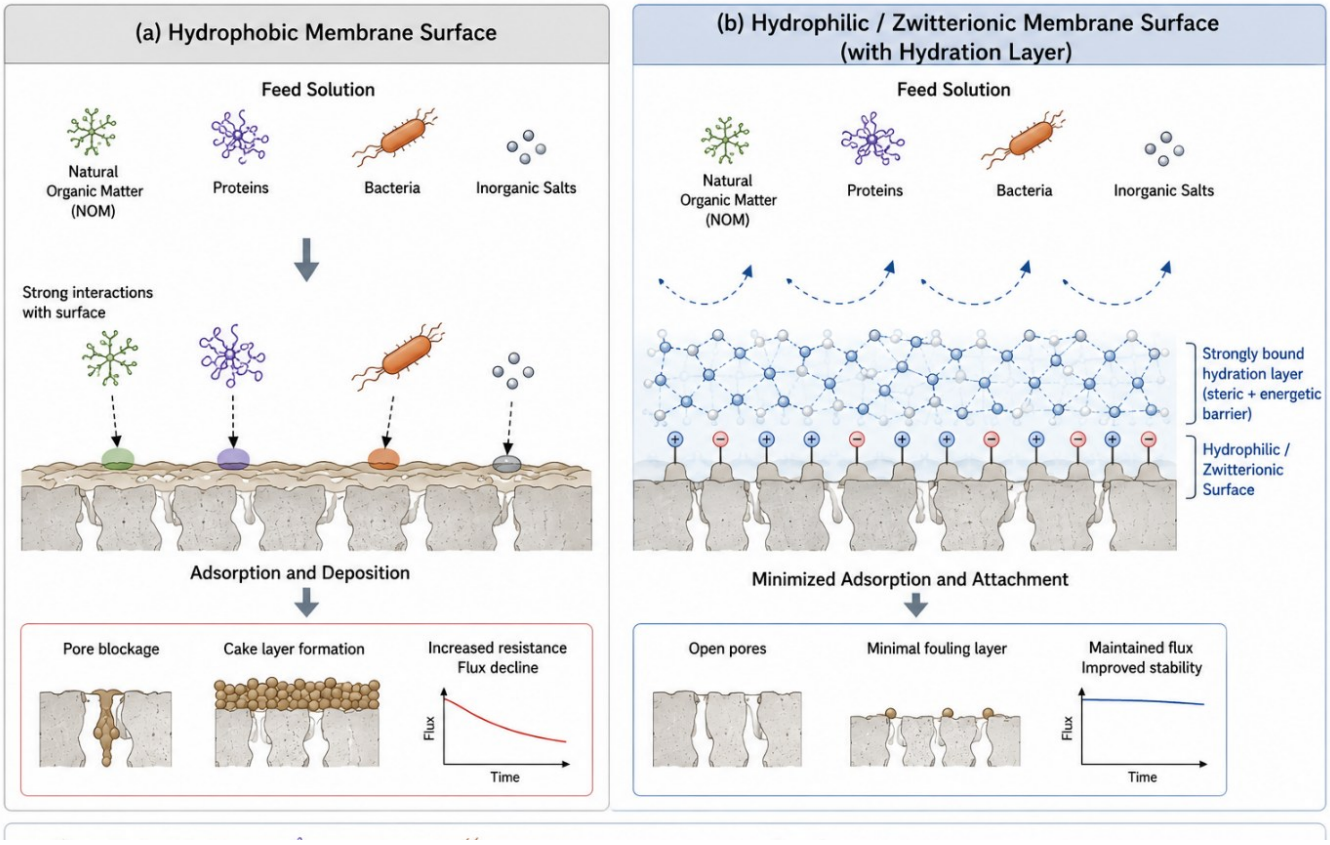

Figure 8. Mechanistic illustration of hydration layer theory for antifouling membranes.

7.5 Advanced Strategies for Mitigating Membrane Fouling

In NF and mixed-matrix membrane systems, fouling remains a persistent challenge that limits the sustainable large-scale application of both pressure-driven and diffusion-controlled separation processes by deteriorating transport performance and selectivity. To address these issues, advanced membrane engineering strategies have been extensively developed to tailor surface chemistry, pore structure, and interfacial properties for improved antifouling performance. Figure 9 graphically presents the different reported strategies currently deployed in the literature.

Among these, structural modification, hydrophilic surface engineering, and plasma-assisted low-temperature functionalization have emerged as highly effective approaches because they directly regulate foulant membrane interactions while preserving or enhancing separation efficiency.

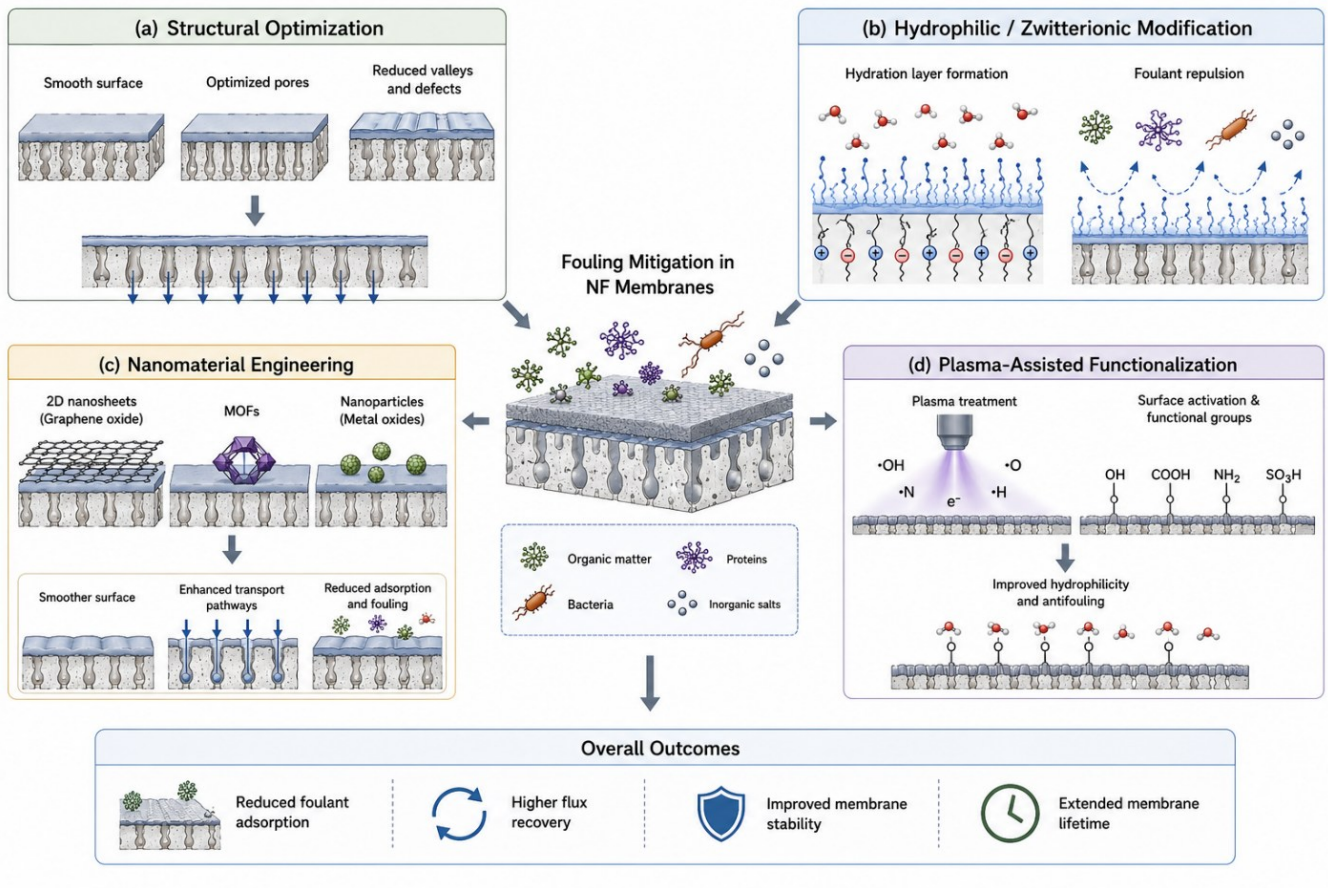

Figure 9. Overview of membrane fouling mitigation approaches: surface structuring, chemical modification, nanomaterial incorporation, and plasma treatment.

7.5.1 Structural Modification of Membrane Materials

Structural modification focuses on redesigning the intrinsic architecture of the membrane matrix to minimize fouling susceptibility. This includes tuning pore size distribution, pore connectivity, surface roughness, porosity, selective layer thickness, and internal free-volume pathways. A well-optimized membrane structure reduces pore blockage and suppresses the entrapment of colloidal and macromolecular foulants. For NF, ultrafiltration (UF), and mixed matrix membranes, incorporation of nanomaterials such as graphene oxide (GO), metal oxides, MOFs, silica nanoparticles, and carbon nanostructures can significantly improve structural uniformity and surface smoothness [114, 115]. These fillers create more controlled transport

pathways and reduce defect sites that often serve as fouling initiation points. In addition, improved mechanical stability prevents compaction-induced pore deformation during long-term filtration. From a mechanistic perspective, structural optimization lowers local concentration polarization, reduces valley-type roughness where foulants accumulate, and facilitates shear-induced foulant removal. In thin-film composite and asymmetric membranes, engineering the support layer morphology is equally important because a highly porous, interconnected support improves back transport of solutes and lowers internal concentration buildup [116]. Collectively, these structural refinements demonstrate that pore architecture and surface roughness are primary design variables linking membrane structure to fouling resistance and sustained flux performance.

7.5.2 Hydrophilic Surface Modification of Membrane Materials

Hydrophilic surface modification is among the most widely employed antifouling strategies because it directly changes the surface–water interaction behaviour. By introducing hydrophilic functional groups such as hydroxyl (–OH), carboxyl (–COOH), amine ($–NH_2$), sulfonic acid ($–SO_3H$), or zwitterionic moieties, the membrane surface develops stronger affinity toward water molecules [117]. This enhanced wettability promotes the formation of a tightly bound hydration layer, which acts as a physical and energetic barrier against the adsorption of proteins, polysaccharides, humic substances, oils, and microbial cells. As a result, foulants experience reduced hydrophobic attraction and weaker van der Waals interactions with the membrane interface. Hydrophilic modification can be achieved through surface grafting, blending with hydrophilic polymers, coating with hydrophilic nanomaterials, or post-functionalization using reactive chemistry. For example, GO-based coatings provide abundant oxygen-containing groups that improve wettability while also enhancing surface smoothness. Similarly, PEGylation and zwitterionic polymer grafting are particularly effective in resisting protein and biofouling due to strong hydration forces. A hydrophilic membrane surface also facilitates cleaning easier and flux recovery because foulant adhesion becomes more reversible. This reinforces surface hydrophilicity as a controllable structural property with direct, measurable consequences for fouling reversibility and operational longevity.

7.5.3 Low-Temperature Plasma-Assisted Surface Functionalization of Membranes

Low-temperature plasma-assisted surface functionalization has emerged as an advanced and highly controllable post-fabrication strategy for membrane antifouling enhancement. This technique utilizes non-thermal plasma generated under mild conditions to activate the membrane surface and introduce reactive species without damaging the bulk polymer matrix. During plasma exposure, energetic ions, radicals, electrons, and UV-active species interact with the membrane surface, generating active sites that enable the incorporation of oxygen-, nitrogen-, or fluorine-containing functionalities [118-120]. This leads to increased hydrophilicity, modified surface charge, enhanced crosslinking density, and controlled surface oxidation. A major advantage of low-temperature plasma treatment is its ability to selectively modify only the top few nanometers of the membrane surface while preserving the original pore structure and bulk mechanical properties. This is especially beneficial for polymeric membranes that are thermally sensitive and unsuitable for high-temperature treatments. In advanced membrane systems, plasma-assisted treatment can also improve nanoparticle anchoring, coating adhesion, and the formation of silica-like ultrathin selective layers under atmospheric pressure conditions. These modifications suppress organic adsorption, reduce bacterial attachment, and improve resistance against irreversible fouling. Because of its solvent-free, rapid, and environmentally friendly nature, plasma-assisted functionalization is increasingly considered a scalable industrial strategy for next-generation antifouling membranes. Overall, this technique exemplifies how nanoscale structural tuning, rather than bulk material replacement, can substantially improve fouling resistance while preserving membrane performance.

Taken together, the fouling mechanisms and mitigation strategies discussed above demonstrate that fouling behaviour in NF and mixed-matrix membranes cannot be understood in isolation from membrane structure. Surface roughness governs foulant nucleation and deposition site availability; hydrophilicity dictates hydration layer stability and foulant reversibility; surface charge modulates electrostatic foulant repulsion; nanofiller incorporation introduces tunable antimicrobial and structural reinforcement effects; and crosslinking density controls the trade-off between fouling resistance and permeance. Rather than treating organic, inorganic, and biological fouling as independent phenomena, these structural parameters represent a unified

design framework through which fouling resistance and long-term operational performance can be systematically engineered in next-generation membranes.

Beyond separation performance and operational stability, next-generation NF membranes must also satisfy environmental and economic requirements. Therefore, structural optimization should not only target improved transport properties but also consider material sustainability, energy consumption, and end-of-life management.

8. Sustainability Assessment of Next-Generation Nanofiltration Membranes

The global membrane market, valued at over USD 28 billion in 2023 and projected to exceed USD 65 billion by 2032, has seen NF membranes emerge as one of its fastest-growing segments, driven by their advantageous properties, including high surface-area-to-volume ratios, tuneable pore architectures, and functional flexibility. [121]. Despite the commercial momentum of nano membranes, systematic sustainability assessment lagged technological development, leaving a critical gap at the edge of materials science and environmental research [122]. Sustainability in the membrane design domain extends three interconnected proportions: environmental impact (energy, emissions, noxiousness); economic viability (CAPEX, OPEX, end-of-life value); and social perspective (occupational health, Transparency in water access, supply chain) [123]. A membrane that is technically excellent, but environmentally/ economically taxing cannot be considered genuinely next generation. Detailed Schematics of the sustainability assessment of next generation nanomembranes is shown in Figure 10.

Recent quantitative LCA and TEA studies indicate that the sustainability of electrospun nanofiber systems is strongly influenced by polymer precursor production, solvent consumption, electrospinning electricity demand, membrane functionalization, and production scale. Evidence from PAN-based electrospun sorbents, PVDF/PVDF-HFP membranes, cellulose nanofibers, and MOF systems highlights the importance of integrating environmental and economic metrics during material and process selection." [123].

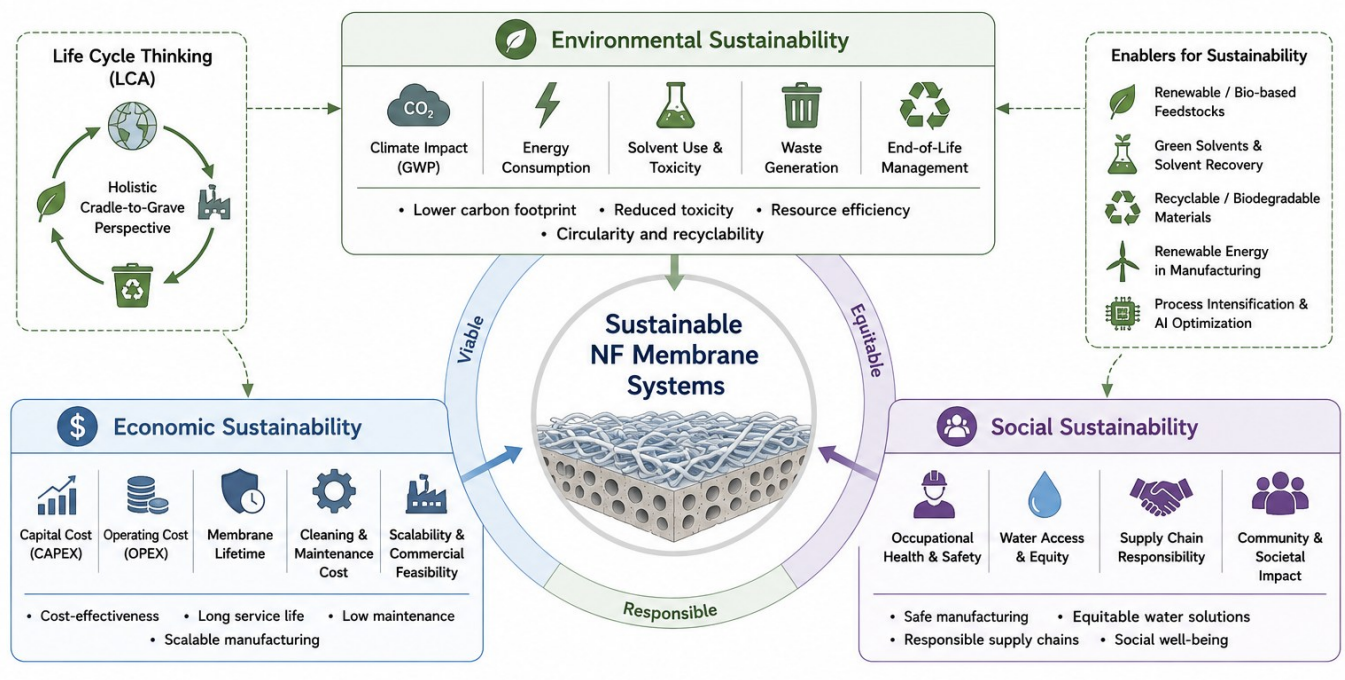

Figure 10. Schematic of life cycle thinking and sustainability framework for NF membrane systems, encompassing environmental, economic, and social dimensions.

8.1 LCA Methodology

LCA, standardized under ISO 14040/44, quantifies environmental impacts from raw material extraction through manufacture, use, and end-of-life. For membrane systems, functional unit selection the quantitative reference for normalizing all environmental burdens is methodologically critical and remains inconsistently applied [125]. Figure 11 present the simplified LCA pathway for analyzing NF membranes. A meta-analysis of 78 membrane LCA studies found that 43% used membrane area, 38% permeate volume, and 19% contaminant removal as functional units, a fragmentation that severely limits cross-study comparison [126]. A compound functional unit (permeate volume per unit area per unit time at a specified rejection threshold) is now gaining acceptance as a standardized basis. System boundary choice is equally consequential: cradle-to-gate assessments dominate early literature but omit the operational phase, which typically represents the largest share of lifecycle energy consumption in water treatment [127].

According to the literature, four environmental hotspots consistently emerge: polymer synthesis (35–60% of global warming potential GWP); solvent use and recovery; electrospinning energy demand (0.8–2.4 kWh/m², two to four times higher than conventional casting); and end-of-life management [128, 129]. PVDF carries a particularly high GWP of 24.8 kg CO_2-eq/m² owing to fluoropolymer chemistry, compared to 9.8 kg CO_2-eq/m² for cellulose acetate [129, 130]. Transitioning to greener solvents such as dimethyl isosorbide or Cyrene has been shown to reduce human toxicity potential by up to 74%, though yield implications must be balanced in the overall assessment [131, 132].

8.2 Comparative Sustainability of Nanofibre Architectures

8.2.1 Bio-derived and Cellulose-Based Systems

Bio-PAN nanofibre membranes synthesized from biomass like sugarcane-derived acrylonitrile exhibit the lowest reported (GWP) global warming potential of 7.3 kg CO_2-eq/m² among high-performance NF-grade nanofibre membranes [133]. Bacterial (CNM) cellulose nanofibre membranes can achieve net negative GWP especially when the biogenic (CS) carbon sequestration during growth is credited and end-of-life (EOL) composting assumed, though results are sensitive to grid electricity mix and end-of-life scenario. Constrained in the scalability of this system are; limited commercial availability of bio-acrylonitrile and 2.5-fold cost premium over petrochemical PAN.

8.2.2 MOF-Functionalized Membranes

MOF incorporated membranes demonstrate high molecular sieving precision and photocatalytic antifouling but besides all of the advantages it introduces significant environmental complexity [134]. The first comprehensive cradle-to-grave LCA reported a GWP of 12.1 kg CO_2-eq/m², with UiO-66 linker synthesis accounting for 44% of total GWP and 61% of freshwater eutrophication potential [135]. A mechanochemical green synthesis pathway is projected to cut GWP by 38%, though scale-up remains to be demonstrated. Covalent anchoring of ZIF-8 to PAN nanofibres via epoxy groups has been shown to reduce zinc leaching to below WHO drinking water guidelines over 1,000 hours of operation [136].

8.3 Graphene Oxide (GO) and 2D Material Systems

GO-enhanced NF membranes achieve water permeance up to 98 L m^{-2} h^{-1} bar^{-1} through frictionless 2D nanochannel transport but GO synthesized from Hummers-method contributes 58% of lifecycle GWP. Graphene oxide synthesized by Electrochemical method reduces GWP by 45% and eliminates the chance of liquid acid waste, representing a critical intervention for the sustainable scale-up of these high-performance systems [137, 138]. Sustainability comparison profile of membrane system is mentioned in Table 3.

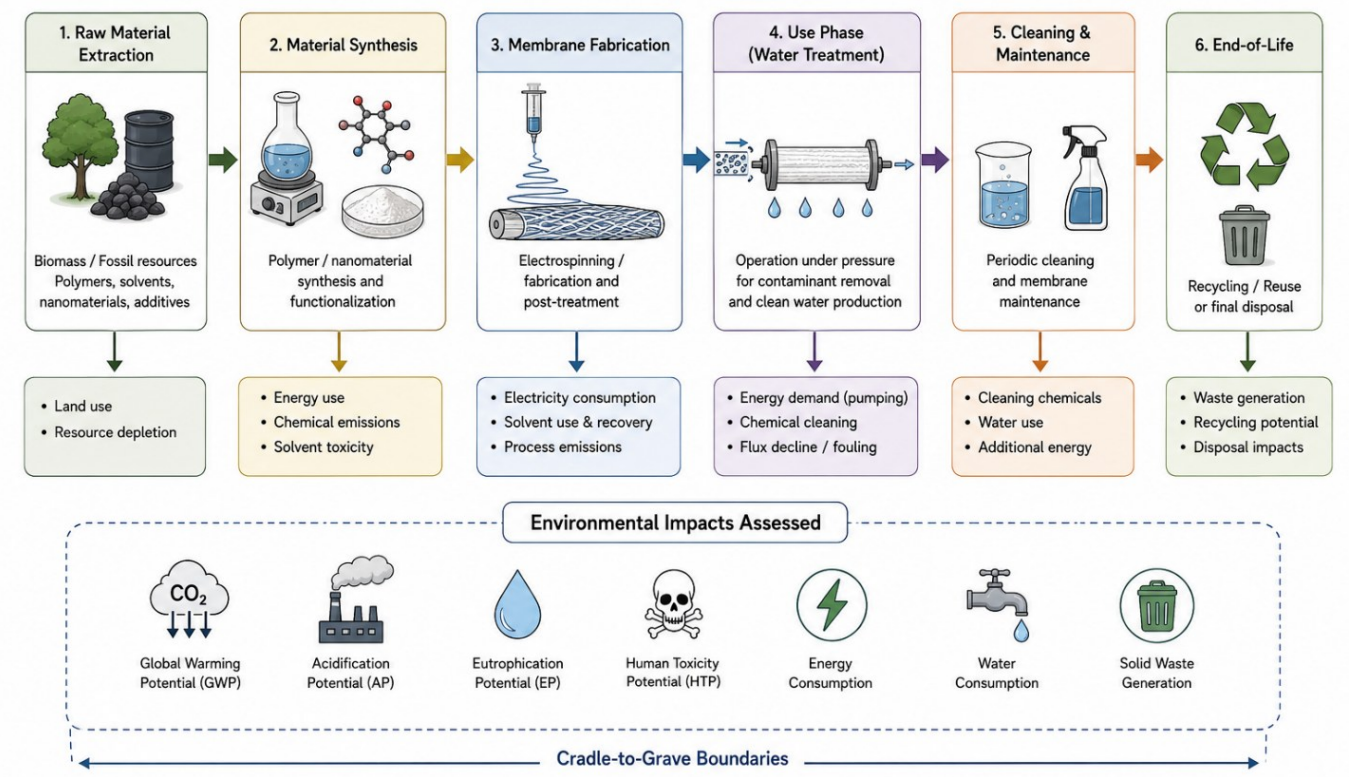

Figure 11. Cradle-to-grave life cycle stages and environmental impact categories for NF membrane systems.

Table 3. A comparative sustainability assessment of six nanofibre membrane architectures and an AI-optimized benchmark.

Membrane System	GWP (kg CO_2-eq/m²)	Energy (kWh/m³)	Key Trade-offs	References
Polyamide TFC (baseline)	18.4	0.42–0.65	High polymerisation energy; non-biodegradable	[125, 126]
Cellulose Acetate NF	9.8	0.30–0.50	Bio-based; moderate hydrolysis stability	[129 - 131]
MOF-Incorporated Nanofibre	12.1	0.28–0.44	Energy savings offset by MOF precursor impacts	[135]
Graphene Oxide (GO) Hybrid	14.6	0.25–0.40	Low operational energy; GO oxidation is carbon-intensive	[137]
Bio-derived PAN Nanofibre	7.3	0.22–0.38	Lowest GWP; bio-PAN scalability constrained	[133]
Recyclable Thermoplastic PES	11.2	0.33–0.55	Closed-loop recyclability; solvent recovery cost	[139]

Global warming potential; TFC = thin-film composite; PES = polyethersulfone; MOF = metal-organic framework.

9. Circular Economy Strategies

Recycling and upcycling strategies for end-of-life polymeric membranes are an important challenge for the sustainable development of membrane-based separation technologies, and a few recent studies focused on recycling and upcycling polymeric membranes have been conducted. The potential of end-of-life poly (ether sulfone) membranes for chemical recovery of valuable products has been demonstrated, with 94.1% of bisphenol S recovery by almost complete hydrolysis of the polymer under optimized conditions using a catalyst [140]. Solvent-based treatment has also been used to recover high-purity polysulfone and

polyester from end-of-life reverse osmosis membranes, demonstrating the potential to recover valuable polymeric components from discarded modules. On the other hand, the used polyvinylidene fluoride (PVDF) membranes have been converted into value-added carbonaceous char (VACC) by optimized pyrolysis at 584 °C for 111 min with a surface area of 344.64 m2/g [141]. Another approach that is being explored is that of a self-healing membrane which can be extended in terms of its function after mechanical damage. Microcapsule-embedded poly (ether sulfone) membranes have shown the recovery of around 103% of their original water flux and 90% of their particle-rejection performance following damage [142].

9.1 Techno-Economic Analysis

Levelized cost of water (LCOW) is the most widely adopted techno-economic analysis metric for membrane water treatment. Across three deployment scales, next-generation nanofibre membranes have been shown to reach cost parity with commercial polyamide TFC membranes at municipal scale when flux exceeds 25 L m^{-2} h^{-1} bar^{-1} and lifetime surpasses 5 years; below these thresholds, LCOW premiums of 35–80% limit competitiveness to premium applications. A critical finding is that TEA models relying on short-term laboratory flux data consistently underestimate OPEX: incorporating 18-month pilot fouling curves increased projected operating costs for bio-derived nanofibre membranes by 28%, driven by additional cleaning frequency and replacement [143].

NF membranes have direct significance to SDGs 6, 12, 13, and 9. Gravity-driven nanofibre membrane systems requiring no energy have demonstrated excellent production of water in pilot deployments in Sub-Saharan Africa and Southeast Asia easily accessible to communities without reliable energy or centralized infrastructure. SDG 12 alignment demands attention to polymer persistence in the ecosystem and microplastic formation hazards, addressable through sustainable biodegradable polymer enhancement [144]. SDG 13 benefits can be achieved through control of pressure drop of NF membranes arise from reduced transmembrane pressure requirements: AI modelling suggests global deployment of next-generation sustainable nanofibre membranes could cut global water sector carbon emissions by 12–18% by 2040 [144].

Inhalation of secondary pollutants during membrane handling raises serious occupational health concerns, with bio-persistence risks like fibre diameter, length, and solubility. Fibres below 3 μm in length are classified as WHO non-respirable, presenting substantially lower respiratory risk [145]. A five-pillar composite sustainability index (CSI) encompassing environmental impact, resource efficiency, economic viability, functional performance, and social responsibility is proposed for structured comparison across architectures [146]. Under stakeholder-derived weights (environmental 30%, performance 25%, economics 20%, resource efficiency 15%, social 10%), bio-derived PAN ranks first overall, followed by cellulose acetate, recyclable PES, AI-optimized hybrids, MOF systems, and GO-enhanced membranes. When performance weighting rises to 40%, AI-optimized hybrids take first place illustrating the sensitivity of rankings to value judgements embedded in the weighting ratios [147].

Significant progress has been made in next generation in the NF and MMMs. These advancements have resulted in membranes that exhibit high permeability and selectivity under controlled laboratory conditions. However, the transition from laboratory-scale innovations to large-scale industrial applications called for a comprehensive assessment of several critical factors [148]. These include materials cost, the scalability of fabrication processes, module compatibility, cleaning and maintenance economics, and potential barriers to commercialization. Such evaluations are crucial for ensuring that these advanced membrane technologies can be effectively integrated into practical systems for water purification, desalination, and various industrial separation processes [149].

Material cost is a critical factor in determining the economic feasibility of NF and MMMs. Conventional NF membranes are typically fabricated from low-cost polymers such as polyamide, supported on substrates like polysulfone or polyethersulfone, benefiting from established manufacturing infrastructure and widespread industrial use [150]. In contrast, next-generation membranes incorporate advanced nanomaterials such as metal–organic frameworks, graphene oxide, carbon nanotubes, and zeolites to enhance permeability, selectivity, and antifouling performance. However, these nanofilters often require complex synthesis methods, expensive precursors, and energy-intensive processing, significantly increasing production costs [151]. Furthermore, the loading level of nanofillers must be carefully optimized, as excessive amounts can lead to aggregation,

interfacial defects, and higher fabrication costs [152]. To address these challenges, current research focuses on developing cost-effective nanomaterials, scalable synthesis techniques, and sustainable fabrication approaches, including the use of green solvents, bio-derived materials, and recyclable fillers to achieve a balance between performance and economic viability as shown in Figure 12.

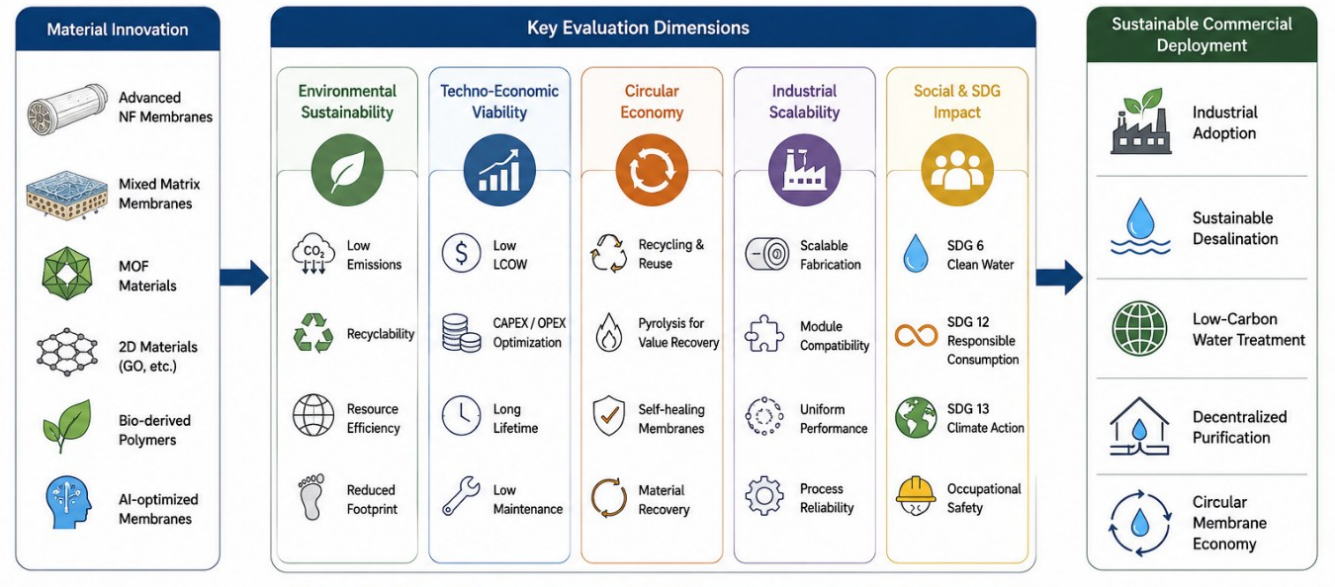

Figure 12. Integrated framework illustrating the pathway toward sustainable commercialization of next-generation NF and MMMs

A major challenge in commercializing advanced NF and MMMs is the scalability of fabrication processes. Many high-performance membranes are produced using laboratory-scale methods such as solution casting, layer-by-layer assembly, and interfacial polymerization, which provide precise structural control but are difficult to scale for industrial production. Industrial manufacturing relies on continuous roll-to-roll processes to produce large membrane sheets with uniform properties. However, maintaining uniform dispersion of nanofillers during scale-up remains a key challenge. Poor dispersion can lead to nanoparticle aggregation, non-selective voids, and reduced mechanical stability, ultimately impairing membrane. Additionally, large-scale production requires strict quality control to ensure consistent thickness, pore structure, and separation efficiency [153]. Variations can lead to performance inconsistencies and increased waste. Therefore, developing scalable fabrication techniques that ensure uniformity, reliability, and cost-effectiveness is essential for successful industrial deployment.

Compatibility with existing membrane module configurations is a key factor in the commercial viability of next-generation membranes. Industrial NF systems commonly use spiral-wound, hollow fibre, and plate-and-frame modules, with spiral-wound designs being the most prevalent due to their high packing density and cost efficiency [154]. Membranes used in these systems must possess adequate mechanical strength, flexibility, and chemical stability to withstand fabrication processes such as rolling, sealing, and bonding [155]. However, MMMs with high nanoparticle loading may become brittle, increasing the risk of cracking or delamination during module assembly or operation. In addition, membranes must endure operational conditions, including pressure, temperature, and chemical exposure. Since NF typically operates at 5–25 bar, strong structural integrity and durability are essential. Ensuring compatibility with existing module designs reduces infrastructure costs and facilitates the industrial adoption of advanced membranes.

Operational and maintenance costs constitute a major portion of the total lifecycle cost of membrane filtration systems. Fouling, scaling, and chemical degradation significantly reduce membrane performance and increase operational expenses [156]. Fouling occurs when organic matter, microorganisms, or inorganic particles accumulate on the membrane surface or within its pores,

causing flux decline and higher energy consumption [157]. To restore performance, periodic cleaning is required, typically using acids, alkaline solutions, and oxidizing agents. These cleaning processes add to operating costs and may gradually degrade membrane materials. Therefore, membranes with enhanced antifouling properties and improved chemical resistance can reduce cleaning frequency and maintenance costs.

Despite promising laboratory-scale performance, several barriers continue to hinder the commercialization of advanced NF and MMM technologies. One major challenge is the formation of interfacial defects between the polymer matrix and nanofillers. Poor compatibility between these components can lead to non-selective voids, particle aggregation, and reduced separation performance [158]. Another limitation is the lack of long-term performance data under realistic operating conditions. Economic uncertainty also affects industrial adoption. Industries often rely on well-established membrane technologies with proven reliability, and introducing new materials requires extensive validation, pilot-scale testing, and regulatory approval. Additionally, concerns about nanoparticle stability and potential leaching may pose environmental and regulatory challenges that slow the commercialization process. Although molecular and material-level innovations determine intrinsic membrane performance, successful implementation requires maintaining these advantages after integration into modules and full-scale systems. Thus, the translation of structure-performance relationships from membrane coupons to industrial operation represents a critical step toward commercialization.

10. From Membrane to Module: System-Level Performance

Moving NF and MMMs from laboratory-scale materials to industrially relevant systems expose a persistent scale-up disconnect. Lab groups routinely optimize pore architecture, surface potential, and filler–matrix adhesion, yet those metrics rarely survive contact with commercial module designs. Once confined within spiral-wound or hollow-fibre housings, membranes encounter non-uniform feed distribution, high packing fractions, and developing concentration gradients that fundamentally rewrite transport behaviour. Indeed, even well-characterized hollow-fibre nanofiltration systems show significant concentration polarization at industrially relevant fibre lengths and recovery rates, where commonly used mass-transfer correlations systematically underpredict the resulting loss in solute retention [159]. The selectivity observed in controlled cross-flow is frequently degraded by boundary layer thickening, pressure-induced compaction, or channeling. Treating the module as a passive container is no longer sufficient; hydrodynamics must be integrated into the membrane design from the outset. Only by mapping the coupling between the intrinsic material selectivity and the flow architecture can we reliably deploy these systems for brine concentration, complex wastewater treatment, or the removal of trace pharmaceuticals, without compromising recovery or long-term stability [160].

10.1 Spiral-Wound Modules

Spiral-wound configurations dominate industrial NF because they pack the highest active area into the smallest footprint. Flat sheets wrapped around a central permeate collector scale linearly, letting plants expand capacity without re-engineering core hydraulics. That efficiency comes with a catch: module output hinges on how the membrane's intrinsic chemistry couples with spacer-driven flow [154]. From a materials perspective, NF and MMM membranes are often designed to achieve precise molecular separations through precise control of pore size and surface chemistry. For example, the incorporation of inorganic fillers into polymer matrices can improve selectivity or permeability by creating preferential transport pathways or by modifying the surface charge [161]. Yet, in spiral-wound modules, these advantages are frequently moderated by concentration polarization. The narrow feed channels, defined by spacers, promote the formation of boundary layers where solutes accumulate near the membrane surface. This localized increase in solute concentration reduces the driving force of permeation which imply a decrease in rejection performance, particularly for multivalent ions or organic micropollutants.

Spacer geometry affects performance in two opposing ways. By breaking up smooth flow and promoting mixing, spacers can reduce concentration polarization and boost mass transfer. But they also raise pressure drop and create low-velocity pockets where material can settle and foul. That compromise is even more important with MMM, whose uneven surfaces, caused by uneven filler distribution or imperfect interfaces, tend to worsen fouling. In wastewater treatment, for example, natural organic

matter and colloids commonly accumulate in those low-shear areas, quickly diminishing module performance. A comparison between the conventional PES membrane and the PES–GO (0.6 wt%) mixed-matrix membrane reveals clear differences in both fouling behaviour and cleaning efficiency [161]. The MMMs exhibited a steeper initial flux decline than the unmodified PES membrane but recovered a substantially higher fraction of its flux after simple hydraulic cleaning, alongside lower protein accumulation in spacer-shadow regions, consistent with its more hydrophilic surface character. This spacer-shadow effect reflects the dual role of feed spacers already established in CFD studies of full-size spiral-wound elements: spacers enhance boundary-layer mixing and mitigate concentration polarization, but simultaneously increase feed-channel pressure loss, so spacer geometry not membrane chemistry alone governs this trade-off.

Thin, selective layers, especially those modified with nanoparticles, are susceptible to gradual compaction under sustained operating pressure, altering effective pore architecture and producing a decline in flux distinct from fouling driven decline, which underscores the need for membranes that retain structural integrity under real-world hydraulic conditions.

However, these limitations do not hinder the widespread use of spiral-wound modules due to their established reliability and ease of incorporation into existing treatment processes. The current challenges involve optimizing the design of spacers, reducing fouling issues, and closely aligning membrane characteristics with hydraulic performance in the module scale, which becomes particularly problematic in novel MMM-based NF modules. Pilot testing with PA-TiO_2 MMMs used in 8-inch spiral wound modules has demonstrated the difficulty in scaling up: the permeation rate of pure water loses about 73% of its value in flat sheets; the salt rejection rate drops 7.7 percentage points; and the critical flux range decreases by 32% [162]. This gap between flat-sheet and module-scale performance is consistent with the concentration-polarization and spacer-hydrodynamic effects established above, where flow non-uniformity along the feed channel not filler chemistry alone governs the inlet-to-outlet performance gradient.

10.2 Hollow Fibre Modules

The hollow fibre arrangement is an architectural design that provides an entirely different way of packaging, with up to 10-30 times more active membrane surface area per unit volume compared to the spiral wound membrane configuration. The design uses thousands of capillary-sized fibres encapsulated in a cylinder housing through which feed is directed from the internal bore to the housing walls or vice versa depending on the tendency to foul and operational pressure [163].

Hollow fibres add more complexities to the relationship between the structure and performance. Variables such as spinning, phase inversion, and subsequent processing affect the internal structure of the fibre, involving the porosity gradient and wall thickness. In the case of MMMs, ensuring uniform distribution of the filler inside the fibre is critical for its performance, but this step poses significant challenges. Failure to ensure uniform distribution or weak interaction may lead to defects, negatively affecting both selectivity and mechanical stability [164]. The hydrodynamic behaviour within hollow-fibre modules differs significantly from that observed in spiral-wound modules. The flow between the tightly packed fibres can be heterogeneous, resulting in variations in velocity and shear stress depending on location. In some areas, dead zones can form due to insufficient flow, causing concentration polarization and fouling.

Fouling resistance in hollow-fibre modules emerges from the interplay between surface energetics and local hydrodynamic shear. Dispersing hydrophilic or antimicrobial fillers within the polymer matrix disrupts foulant adhesion kinetics, delivering measurable fouling mitigation in complex aqueous matrices like municipal wastewater and pharmaceutical effluents. For instance, hollow-fibre MMMs incorporating 0.5 wt% graphene oxide have demonstrated 15–22% higher flux recovery ratios and ~30% lower irreversible fouling resistance compared to neat polymer controls when filtering secondary wastewater effluent[165]; similarly, Ag-doped MMMs reduced biofilm attachment by >40% in pharmaceutical process water trials[166].

The fouling behaviour in HF modules is dependent on surface chemistry and hydrodynamics. Although hydrophilic/antimicrobial MMMs prevent fouling by reducing attachment of foulants in wastewater and pharmaceutical systems, the efficiency is less in areas with low shear and no fluid motion. Despite their advantages, which include frequent backflushing and chemical cleaning

for increased lifetime and lower pumping requirements, mechanical weakness, flow distribution issues, and problems with scaling remain limitations to pressurized NF processes. Flow distribution within the fibre bundle is an independently modeled source of module-scale performance loss: three-dimensional CFD simulations coupling shell-side and lumen-side flow with the permeation and fouling behaviour of industrial hollow-fibre modules show that non-uniform flow across the bundle directly shapes local fouling development, a scale-dependent effect absent from single-fibre lab characterization, consistent with the broader lab-to-full-scale performance gaps reported for hollow-fibre nanofiltration

The performance of a module is often determined by hydrodynamics, which can sometimes overshadow the membrane's intrinsic properties. The interaction between flow regime, shear stress, and module geometry governs mass transfer processes. This interaction influences both flux and rejection [167]. In many NF systems, flow conditions are predominantly laminar because of the small channel dimensions. Consequently, concentration polarization emerges as a substantial constraint. The membrane surface is where solutes build up, leading to an increase in local osmotic pressure and a decrease in permeate flux. For MMMs, where selective transport mechanisms may rely on specific interactions between solutes and embedded fillers, this effect can alter separation performance in non-trivial ways [168].

Increasing crossflow velocity is a strategy to mitigate concentration polarization by enhancing shear stress and thinning the boundary layer. However, this approach is not without drawbacks. Higher velocities lead to increased energy consumption. They may also exacerbate pressure drop across the module. In spiral-wound systems, spacer-induced turbulence can partially address this issue, but at the cost of additional hydraulic resistance. Achieving uniform shear stress across all fibres in hollow fibre modules remains a persistent challenge [169].

The relationship between hydrodynamics and fouling is also complicated. Fouling is influenced not only by membrane surface properties but also by the transport and deposition of particles within the flow field. Low-shear regions tend to favor the accumulation of foulants, while high-shear may delay deposition but can also compact fouling layers once they have formed [170]. MMMs introduce another layer of complexity because changes in surface roughness and chemistry induced by fillers can modify interactions with foulants. The evidence is substantial and specific. The lab-to-module performance discrepancy has been directly demonstrated using a CFD model to establish relationships between membrane properties and module-scale performance [171]. Geometric effects during upscaling have been quantified, showing that wavy channels and spacers achieved 35–40% flux improvements at higher Reynolds numbers [172]. Concentration polarization has been identified as a critical scale-up limitation, with design solutions such as baffles proposed for gas recirculation. Performance has been shown to drop significantly in scaled modules (1 m length), with scaling occurrence dependent on temperature and flow conditions [173]. These approaches provide valuable insights. They show how advanced membrane materials can be effectively integrated into large-scale systems.

10.3 Industrial Challenges and Constraints: From Membrane to Module

Next-generation NF and MMMs have made measurable progress in permeability, selectivity, and antifouling performance. Yet converting those laboratory gains into reliably operating industrial modules is a challenge that materials science alone cannot resolve. The barriers are layered and interconnected: fouling erodes flux and elevates energy costs; filler–polymer incompatibility undermines selectivity; module assembly introduces defects absent from flat-sheet coupons; and the economics of high-performance nanocomposite membranes remain formidable [174]. The inverse relationship between flux and rejection is the defining design constraint for all dense membranes. Incorporating nanofillers MOFs, graphene oxide, functionalized nanosheets to push permeance beyond conventional thin-film composite (TFC) baselines demand precise control of filler loading and pore architecture; when that control is lost, selectivity declines or mechanical integrity is compromised. Recent work has approached this limit from new directions: a polyamide network formed by polymerization of a quaternized-spiro piperazine and TMC achieved an increase in free fractional volume owing to enhanced monomer rigidity, yielding a permeance of approximately 22 L $m^{-2}\cdot h^{-1}\cdot bar^{-1}$ [10], yet laboratory demonstrations of this kind rarely include performance data under extended operation with realistic feed chemistry, which is precisely what industrial operators require before committing capital.

Fouling remains the most consequential operational challenge for industrial NF as shown in Figure 13. A rigorous economic analysis of seven full-scale NF and RO installations in the Netherlands found that fouling-related costs constituted roughly 11% of operational expenditure (OPEX) for NF plants fed on anoxic groundwater, compared with approximately 24% for RO plants treating surface water or municipal effluent, with premature membrane replacement identified as the dominant cost driver in both cases [175]. This gap is meaningful: NF is genuinely less fouling-intensive under favorable feed conditions, but the advantage disappears when feed quality deteriorates.

At engineering-scale drinking water treatment plants monitored over multi-year horizons, continuous NF operation has been shown to double NF concentrate (NFC) yield while causing a 30% decline in chloride retention, with the rejection of total hardness and sulphate comparatively unaffected [176] . A study following a two-stage engineering NF project for municipal drinking water treatment over six months found that inorganic fouling dominated both stages driven by deposition of aluminum, calcium, and silicon , while humic acid-like compounds and phosphorus were abundant in the fouling layer at each stage despite pronounced spatial differences between them [177].The implication is direct: single-foulant bench tests cannot reproduce this chemical complexity, and laboratory antifouling results consistently overpredict field performance. For MMMs specifically, surface heterogeneity from partially exposed inorganic fillers creates additional nucleation sites; studies on electro spun GO–ZnO/polysulfone MMMs demonstrated that the pristine polysulfone baseline exhibited markedly lower flux recovery relative to the nanocomposite membranes, confirming that filler selection critically governs antifouling stability under pressure cycling [178].The central fabrication challenge of MMMs achieving defect-free filler dispersion across industrially relevant membrane areas originates in the fundamental physicochemical mismatch between hydrophilic inorganic fillers (zeolites, MOFs, graphene oxide, MXenes) and hydrophobic engineering polymers such as polysulfone and polyethersulfone. Inter-filler agglomeration generates “sieve-in-a-cage” voids that allow solutes to bypass the selective layer, degrading both selectivity and mechanical properties simultaneously.

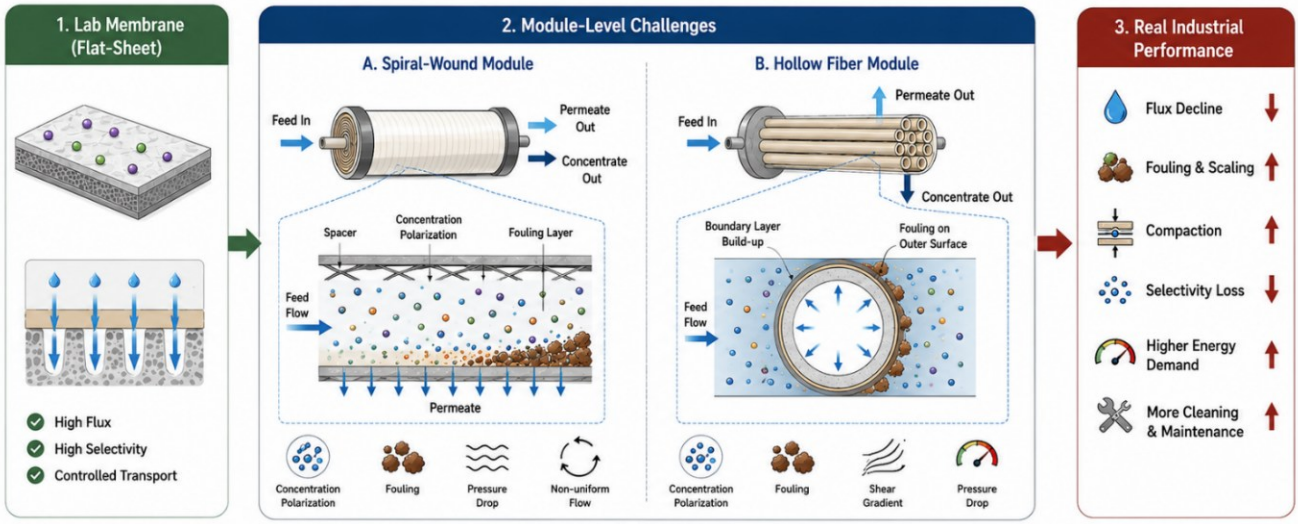

Figure 13. Conceptual framework illustrating the transition from laboratory-scale NF and MMMs to industrial module-scale performance

A practical illustration of how far the frontier lies: fabricating PVAm/ZIF-8/modified polysulfone MMMs with effective areas up to 3,100 cm² and selective layers of approximately 200 nm required a dedicated vacuum sintering strategy, setting a high bar for MMMs material premiums to overcome. Spiral wound modules carry average operational lifespans of 5–10 years, and by 2025 approximately 30,000 tons of spent elements will have been generated globally, with no satisfactory circular economy pathway yet in place [179].

NF systems at drinking water treatment plants typically operate at 40–60% water recovery [164]. Economic and environmental constraints further restrict industrial deployment. The high costs associated with advanced nanomaterials, solvent-less fabrication equipment, and module fabrication must be balanced against performance gains to ensure commercial viability. In addition, sustainability regulations drive efforts to replace toxic solvents with greener alternatives and to minimize waste during membrane manufacture, motivating the development of biodegradable polymers and solvent-free fabrication routes [180]. At the module level, scaling up the performance of membranes involves addressing difficulties in sealing, pressure, and optimal mass transport to prevent concentration polarization. This pressure and flow related cost is significant in its own right: the same economic analysis of full-scale NF and RO plants identified increased feed channel pressure drop and permeability loss, independent of membrane replacement, as core components of operational expenditure, underscoring that hydrodynamic degradation carries a real cost distinct from chemical fouling [175] Novel membrane designs incorporating NF with other techniques such as electrodialysis appear promising as a means of improving both selectivity and flux, especially in areas such as lithium extraction from salt-lake brines, where effective separation of Mg^{2+}/Li^{+} is paramount [181]. Nevertheless, engineering and economic factors have constrained the broad application of such novel membranes in industry.

Even when advanced NF membranes demonstrate promising technical performance, their industrial adoption depends on meeting safety, environmental, and regulatory requirements. Regulatory considerations therefore represent an external constraint that influences material selection, fabrication strategies, and practical deployment.

11. Regulatory Challenges and Constraints

Compliance with regulatory requirements on the manufacturing of the new generation of NF and MMMs covers the entire cycle from membrane manufacturing through membrane modules integration and is based on international standards related to quality management (ISO 9001), environmental management (ISO 14001), and environmentally sound chemical management (REACH). In the process of membrane manufacturing, reproducibility, reduction of defects, and effective interfacial engineering should be ensured, especially in cases of MMMs in which the interaction between the inorganic particles, MOF or green synthesized nanoparticles, in particular, and the polymer matrix play a pivotal role, since in case of inadequate interfacial properties, agglomeration and interfacial defects will be inevitable [181, 182]. Industry guidelines emphasize thorough characterization using SEM, FTIR, and AFM to detect defects, confirm filler distribution, and validate membrane morphology, which are essential for certification and operational guarantees [183].

Compliance for manufacturing next-generation NF and MMMs spans the entire cycle, from membrane synthesis through module integration, and is governed by a combination of mandatory regulation and voluntary certifiable standards. Chemical safety is subject to mandatory regulatory frameworks such as the EU's REACH regulation (EC No 1907/2006) [182], which governs the registration, evaluation, and authorization of chemical substances placed on the market. Separately, manufacturers may pursue voluntary certification against ISO 9001:2015 for quality management [183] and ISO 14001:2026 for environmental management [184] to demonstrate process consistency and environmental responsibility. In the process of membrane manufacturing, reproducibility, reduction of defects, and effective interfacial engineering should be ensured, especially in cases of MMMs in which the interaction between the inorganic particles, MOF or green synthesized nanoparticles, in particular, and the polymer matrix play a pivotal role, since in case of inadequate interfacial properties, agglomeration and interfacial defects will be inevitable [181, 185]. Industry guidelines emphasize thorough characterization using SEM, FTIR, and AFM to detect defects, confirm filler distribution, and validate membrane morphology, which are essential for certification and operational guarantees [186]

Environmental safety and sustainability add another layer of complexity that the industry is actively grappling with. The growing shift toward biodegradable polymers, safer additives like chitosan, biochar, and bio-ionic liquids, and greener synthesis approaches such as using Hibiscus rosa-sinensis to produce silver nanoparticles reflects a genuine effort to move away from hazardous chemicals and reduce environmental impact across every stage of a membrane’s lifecycle [186-188]. To ensure sustainability of the development project, regulations call for strict toxicology tests, effects on water, soil, and air quality evaluations, and lifecycle assessment studies to ensure that the development is truly sustainable [189].

The certification protocol is indeed very stringent in terms of the necessary tests carried out to assess the performance, longevity, chemical stability, and antifouling properties of the membranes prior to their commercialization [190]. It is important to conduct such tests under conditions of practical operations, which include processes like desalination or CO_2 capture. The module design, on the other hand, needs to satisfy certain criteria related to the pressure safety, chemical compatibility, tight seal, and consistent production in a large-scale setting [191], whereas characterization using SEM, FTIR, and AFM techniques is essential in terms of ensuring that the membrane does not suffer from any defects and has the required morphology. There are also issues of managing nanomaterials within the process, which require compliance with the relevant OH&S laws in relation to the containment, handling, storage, and disposal of MOFs and silver nanoparticles. Addressing this disconnect requires the membrane research community, standards bodies, and regulators to build shared governance frameworks specifically designed for next-generation nanocomposite membrane systems.

The core trade-off is that improving permeability usually compromises selectivity. Adding nanofillers to push performance further only works when filler distribution is tightly controlled. When that control is lost, the membrane either stops separating properly or loses its mechanical integrity. Fouling compounds everything: real-world feed streams carry a mixture of organic matter, inorganic deposits, proteins, and colloids that bench-scale tests simply cannot replicate, so laboratory antifouling results routinely overestimate field performance. Moving from a flat sheet in a lab to an actual module is where gains most often disappear. Spiral-wound and hollow-fibre configurations introduce concentration polarization, uneven flow, and pressure compaction that never appear in controlled testing. Hydrodynamics, including flow regime, shear stress, and channel geometry, often govern final performance more than the membrane material itself. On the regulatory side, compliance spans the full lifecycle covering fabrication standards, nanomaterial handling, toxicology testing, and end-of-life disposal. The industry is moving toward greener materials and safer solvents, but large volumes of spent membrane elements continue to accumulate with no established recycling pathway in place.

12. Future Research Directions

Future research should focus on establishing quantitative structure–transport–performance relationships that link molecular architecture, interfacial polymerization kinetics, membrane morphology, and module-scale operation. A deeper understanding of polymer–filler interphase physics, defect formation mechanisms, and nanochannel transport will be critical for improving performance, selectivity, and long-term stability of mixed-matrix and thin-film nanocomposite membranes.

To reduce reliance on empirical optimization, advanced characterization techniques should be integrated with molecular simulations, multiscale modelling, and machine learning approaches. AI-driven frameworks, including physics-informed models, digital twins, and autonomous experimentation, offer strong potential for accelerating membrane discovery and enabling predictive process optimization.

Bridging the gap between laboratory and industrial performance will require long-term evaluation under realistic operating conditions, with emphasis on fouling behaviour, concentration polarization, membrane compaction, hydrodynamics, and operational stability in pilot- and full-scale systems. Efforts are also needed to develop scalable fabrication strategies, improve module design, and ensure compatibility with existing membrane configurations.

Lastly, sustainability should be a central design principle in next-generation NF membrane development. Emphasis should be placed on green synthesis routes, recyclable and biodegradable materials, low-energy fabrication processes, lifecycle assessment, and circular economy strategies to ensure that future NF systems are both high-performing and environmentally responsible.

13. Conclusions

This review has presented a comprehensive analysis of the structure–performance relationships governing next-generation nanofiltration (NF) membranes by integrating molecular architecture, nanostructuring strategies, interfacial engineering, transport mechanisms, fouling behaviour, artificial intelligence, sustainability, and system-level deployment within a unified

multiscale framework. Significant progress has been achieved through advances in monomer engineering, free-volume regulation, interfacial polymerization, and nanomaterial incorporation. Macrocyclic monomers, metal–organic frameworks (MOFs), covalent organic frameworks (COFs), graphene oxide, MXenes, and other nanostructured materials have significantly expanded the design space of NF and mixed-matrix membranes by enabling tailored nanochannels with improved permeability, selectivity, and antifouling properties.

Meanwhile, advances in multiscale modelling, molecular simulations, machine learning, and AI-assisted membrane design have provided new opportunities for predictive structure optimization and accelerated membrane discovery. In parallel, the integration of green synthesis strategies, lifecycle assessment, and circular economy concepts has highlighted the importance of developing more sustainable membrane technologies.

Despite these advances, several critical challenges continue to restrict practical deployment. The complex coupling between membrane chemistry, interfacial polymerization kinetics, nanoscale morphology evolution, and ion transport mechanisms remains insufficiently understood, limiting the ability to achieve fully predictive membrane design. Moreover, interfacial defects, nanofiller dispersion issues, concentration polarization, membrane compaction, fouling under realistic feed conditions, and module-scale hydrodynamic limitations remain major obstacles to maintaining long-term performance. Beyond scientific challenges, large-scale commercialization is constrained by scalable manufacturing, material cost, process reproducibility, regulatory requirements, and insufficient pilot-scale demonstration.

Moving forward, several key principles should guide the development of next-generation NF membranes:

1) Precise regulation of nanoscale structural parameters is fundamental for performance enhancement. Membrane pore size distribution, surface charge density, free volume, selective-layer thickness, crosslinking degree, and interfacial architecture are the primary structural factors determining permeability, selectivity, and stability. Future efforts should focus on establishing quantitative structure-performance relationships rather than relying on empirical material screening.
2) The major scientific bottleneck remains overcoming the permeability-selectivity-stability trade-off. Although advanced materials have achieved impressive laboratory-scale performance, maintaining selective transport while ensuring mechanical robustness, chemical stability, and resistance to fouling under realistic operating conditions remains unresolved.
3) The most significant barriers to industrial translation are scalability, reproducibility, and economic viability. Many emerging membrane materials rely on complex synthesis procedures, expensive precursors, or laboratory-specific fabrication conditions. Future research should prioritize scalable fabrication routes, environmentally benign materials, simplified manufacturing processes, and comprehensive techno-economic evaluations.
4) Predictive design approaches will be essential for accelerating membrane innovation. The integration of advanced characterization, molecular simulations, transport modelling, and AI-driven approaches can provide deeper mechanistic understanding and enable rational design of membranes with targeted separation functions.
5) Future NF technologies should shift from performance-driven materials development toward application-oriented membrane systems. Practical success will require simultaneous consideration of separation efficiency, energy consumption, fouling control, environmental impact, module integration, and long-term operation in real industrial environments.

The future of NF membrane technology will depend on bridging the gap between molecular-scale innovation and engineering-scale implementation. An integrated framework combining advanced materials design, predictive modelling, sustainable manufacturing, and system-level optimization will be essential for developing highly selective, energy-efficient, fouling-resistant, scalable, and environmentally sustainable NF platforms for water treatment and resource recovery applications.

Conflict of Interest

The authors declare no conflict of interest related to the publication of this research.

Data Availability Statement

No new data were created or analyzed in this study.

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References

[1] M. S. Mauter, I. Zucker, F. Perreault, J. R. Werber, J. H. Kim, and M. Elimelech, "The role of nanotechnology in tackling global water challenges," Nature Sustainability 2018 1:4, vol. 1, no. 4, pp. 166-175, Apr. 2018, https://doi.org/10.1038/s41893-018-0046-8

[2] M. Elimelech and W. A. Phillip, "The future of seawater desalination: Energy, technology, and the environment," Science (1979)., vol. 333, no. 6043, pp. 712-717, Aug. 2011, https://doi.org/10.1126/science.1200488

[3] Y. Zhao, T. Tong, X. Wang, S. Lin, E. M. Reid, and Y. Chen, "Differentiating Solutes with Precise Nanofiltration for Next Generation Environmental Separations: A Review," Environ. Sci. Technol., vol. 55, no. 3, pp. 1359-1376, Feb. 2021, https://doi.org/10.1021/acs.est.0c04593

[4] H. Wen and J. P. Chen, "Molecular engineering strategies for high-performance polyamide nanofiltration membranes: A review," Chemical Engineering Journal, vol. 533, p. 174486, Apr. 2026, https://doi.org/10.1016/j.cej.2026.174486

[5] S. LOEB and S. SOURIRAJAN, "Sea Water Demineralization by Means of an Osmotic Membrane," pp. 117-132, Jan. 1963, https://doi.org/10.1021/ba-1963-0038.ch009

[6] J. E. Cadotte, R. J. Petersen, R. E. Larson, and E. E. Erickson, "A new thin-film composite seawater reverse osmosis membrane," Desalination, vol. 32, no. C, pp. 25-31, Jan. 1980, https://doi.org/10.1016/S0011-9164(00)86003-8

[7] J. E. Cadotte, R. S. King, R. J. Majerle, and R. J. Petersen, "Interfacial Synthesis in the Preparation of Reverse Osmosis Membranes," Journal of Macromolecular Science-Chemistry, vol. 15, no. 5, pp. 727-755, 1981, https://doi.org/10.1080/00222338108056764

[8] W. J. Lau, A. F. Ismail, N. Misdan, and M. A. Kassim, "A recent progress in thin film composite membrane: A review," Desalination, vol. 287, pp. 190-199, Feb. 2012, https://doi.org/10.1016/j.desal.2011.04.004

[9] B. Wu et al., "Custom-tailoring zwitterion-based nanofiltration membranes for organic molecule desalination with sub-200 Da molecular weight," J. Memb. Sci., vol. 698, p. 122585, Apr. 2024, https://doi.org/10.1016/j.memsci.2024.122585

[10] H. Peng, K. Yu, X. Liu, J. Li, X. Hu, and Q. Zhao, "Quaternization-spiro design of chlorine-resistant and high-permeance lithium separation membranes," Nat. Commun., vol. 14, no. 1, pp. 5483-, Dec. 2023, https://doi.org/10.1038/s41467-023-41169-x

[11] Y. Xu, H. Peng, H. Luo, Q. Zhang, Z. Liu, and Q. Zhao, "High performance Mg2+/Li+ separation membranes modified by a bis-quaternary ammonium salt," Desalination, vol. 526, p. 115519, Mar. 2022, https://doi.org/10.1016/j.desal.2021.115519

[12] W. Zhang et al., "Lignin alkali regulated interfacial polymerization towards ultra-selective and highly permeable nanofiltration membrane," Nature Communications 2025 16:1, vol. 16, no. 1, pp. 371-, Jan. 2025, https://doi.org/10.1038/s41467-024-55595-y

[13] Q. Peng et al., "Extreme Li-Mg selectivity via precise ion size differentiation of polyamide membrane," Nature Communications 2024 15:1, vol. 15, no. 1, pp. 2505-, Mar. 2024, https://doi.org/10.1038/s41467-024-46887-4

[14] Z. Ali, J. Bai, W. Ali, M. Hassan, L. Shan, and X. Zhang, "Host-guest assembly engineered nanofiltration membrane for high-efficiency ion-ion separation," AIChE Journal, vol. 72, no. 5, p. e70251, May 2026, https://doi.org/10.1002/aic.70251

[15] H. Fan, M. Peng, I. Strauss, A. Mundstock, H. Meng, and J. Caro, "MOF-in-COF molecular sieving membrane for selective hydrogen separation," Nature Communications 2021 12:1, vol. 12, no. 1, pp. 38-, Jan. 2021, https://doi.org/10.1038/s41467-020-20298-7

[16] A. Anand, B. Unnikrishnan, J. Y. Mao, H. J. Lin, and C. C. Huang, "Graphene-based nanofiltration membranes for improving salt rejection, water flux and antifouling-A review," Desalination, vol. 429, pp. 119-133, Mar. 2018, https://doi.org/10.1016/j.desal.2017.12.012

[17] X. Han, X. Qiu, M. Zong, and J. Hao, "Assembled MXene Macrostructures for Multifunctional Polymer Nanocomposites," Small Struct., vol. 4, no. 10, p. 2300090, Oct. 2023, https://doi.org/10.1002/sstr.202300090

[18] B. Sengupta et al., "Carbon-doped metal oxide interfacial nanofilms for ultrafast and precise separation of molecules," Science (1979)., vol. 381, no. 6662, pp. 1098-1104, Sep. 2023, https://doi.org/10.1126/science.adh2404

[19] J. Cui et al., "Tailored poly(ionic liquid) nanofiltration membrane for efficient Li+/Mg2+ separation," Sep. Purif. Technol., vol. 394, Jul. 2026, https://doi.org/10.1016/j.seppur.2026.137412

[20] A. Abdulsalam et al., "A review of fouling prediction techniques in membrane desalination: From empirical to intelligent models," Desalination, vol. 616, Dec. 2025, https://doi.org/10.1016/j.desal.2025.119363

[21] J. Luo and Y. Wan, "Effects of pH and salt on nanofiltration-a critical review," J. Memb. Sci., vol. 438, pp. 18-28, Jul. 2013, https://doi.org/10.1016/j.memsci.2013.03.029

[22] C. Jiang et al., "Ultrathin Film Composite Membranes Fabricated by Novel in Situ Free Interfacial Polymerization for Desalination," ACS Appl. Mater. Interfaces, vol. 12, no. 22, pp. 25304-25315, Jun. 2020, https://doi.org/10.1021/acsami.0c05166

[23] M. M. Jia et al., "Deciphering the role of camphor sulfonic acid and triethylamine in Thin-Film composite reverse osmosis membranes for water desalination," Sep. Purif. Technol., vol. 369, p. 133136, Oct. 2025, https://doi.org/10.1016/j.seppur.2025.133136

[24] T. Huang, M. Alyami, N. M. Kashab, and S. P. Nunes, "Engineering membranes with macrocycles for precise molecular separations," J. Mater. Chem. A Mater., vol. 9, no. 34, pp. 18102-18128, Aug. 2021, https://doi.org/10.1039/D1TA02982G

[25] C. Jiang, S. Bai, J. Li, M. Wang, Y. Zhou, and Y. Hou, "Crown ether-functionalized nanofiltration membranes with high ions selectivity for Li+/Mg2+ separation," J. Memb. Sci., vol. 714, p. 123372, Jan. 2025, https://doi.org/10.1016/j.memsci.2024.123372

[26] H. Zhang et al., "Carboxyl-functionalized graphene oxide polyamide nanofiltration membrane for desalination of dye solutions containing monovalent salt," J. Memb. Sci., vol. 539, pp. 128-137, 2017, https://doi.org/10.1016/j.memsci.2017.05.075

[27] X. Wang, K. Yang, H. Xu, Y. Huang, C. Gao, and X. Gao, "Incorporating functionalized acyl chloride monomer with rigid pyrrolidinyl group via two-step interfacial polymerization for improving permeability of reverse osmosis membranes," Desalination, vol. 565, Nov. 2023, https://doi.org/10.1016/j.desal.2023.116880

[28] Y. Shen et al., "Deciphering the Structure-Performance Relationship of Polyamide Organic Solvent Nanofiltration Membranes via Synergistic Control of Monomer Geometry and Functionality," Adv. Funct. Mater., p. e31403, 2026, https://doi.org/10.1002/adfm.202531403

[29] H. Ding, M. Huang, Y. Liu, L. Zhang, H. Pei, and X. Li, "Mediated regulation of interfacial polymerization diffusion by 18-crown-6-ether: A fabrication strategy for high-performance nanofiltration membranes," J. Memb. Sci., vol. 728, Jun. 2025, https://doi.org/10.1016/j.memsci.2025.124102

[30] Y. Sun, M. Yan, Z. Li, L. Wang, X. Chen, and S. Luo, "Diffusion-Regulated Interfacial Polymerization of Hierarchically Microporous Polyamide Membranes for Permselective Gas Separations," ACS Appl. Mater. Interfaces, vol. 16, no. 38, pp. 51532-51541, Sep. 2024, https://doi.org/10.1021/acsami.4c10941

[31] Y. Liang et al., "Polyamide nanofiltration membrane with highly uniform sub-nanometre pores for sub-1 Å precision separation," Nature Communications 2020 11:1, vol. 11, no. 1, pp. 2015-, Apr. 2020, https://doi.org/10.1038/s41467-020-15771-2

[32] S. Karan, Z. Jiang, and A. G. Livingston, "Sub-10 nm polyamide nanofilms with ultrafast solvent transport for molecular separation," Science (1979)., vol. 348, no. 6241, pp. 1347-1351, Jun. 2015, https://doi.org/10.1126/science.aaa5058

[33] Z. Tan, S. Chen, X. Peng, L. Zhang, and C. Gao, "Polyamide membranes with nanoscale Turing structures for water purification," Science (1979)., vol. 360, no. 6388, pp. 518-521, May 2018, https://doi.org/10.1126/science.aar6308

[34] Z. Wang et al., "Nanoparticle-templated nanofiltration membranes for ultrahigh performance desalination," Nature Communications 2018 9:1, vol. 9, no. 1, pp. 2004-, May 2018, https://doi.org/10.1038/s41467-018-04467-3

[35] X. Zhu et al., "Crumple-textured polyamide membranes via MXene nanosheet-regulated interfacial polymerization for enhanced nanofiltration performance," J. Memb. Sci., vol. 635, p. 119536, Oct. 2021, https://doi.org/10.1016/j.memsci.2021.119536

[36] H. Zhang et al., "Crumpled polyamide membranes templated by macroporous scaffolds for ultra-permeable nanofiltration," Desalination, vol. 612, p. 118958, Oct. 2025, https://doi.org/10.1016/j.desal.2025.118958

[37] Z. Qiu, H. Han, T. Wang, R. Dai, and Z. Wang, "Nanofoaming by surfactant tunes morphology and performance of polyamide nanofiltration membrane," Desalination, vol. 552, p. 116457, Apr. 2023, https://doi.org/10.1016/j.desal.2023.116457

[38] C. Zhao et al., "Polyamide membranes with nanoscale ordered structures for fast permeation and highly selective ion-ion separation," Nature Communications 2023 14:1, vol. 14, no. 1, pp. 1112-, Feb. 2023, https://doi.org/10.1038/s41467-023-36848-8

[39] Y. K. Wang et al., "A Review on Monomer Design for Interfacial Polymerization: Bridging Liquid Separation and Gas Separation Membranes," Sep. Purif. Technol., vol. 394, Jul. 2026, https://doi.org/10.1016/j.seppur.2026.137593

[40] X. Zhang, P. Choi, N. K. Khanzada, P. W. Wong, and K. An, "Highly Permeable Chlorine-Resistant Forward Osmosis Membrane by Grafting Novel Sulfonamide Monomers," SSRN Electronic Journal, 2023, https://doi.org/10.2139/ssrn.4408161

[41] J. Alom et al., "Covalent Organic Framework (COF) based mixed matrix membranes as an alternative solution for gas separation," J. Memb. Sci., vol. 753, p. 125620, Jul. 2026, https://doi.org/10.1016/j.memsci.2026.125620

[42] M. Alsaady, S. Waqas, M. A. Almarshoud, K. Maqsood, A. Abdulrahman, and Y. Yan, "Polysulfone/Graphene Oxide Mixed Matrix Membranes for Improved CO2/CH4 Separation," Membranes 2025, Vol. 15, Page 386, vol. 15, no. 12, p. 386, Dec. 2025, https://doi.org/10.3390/membranes15120386

[43] S. Cong et al., "Designing and construction of 2D MXene membranes for advanced separation," Sep. Purif. Technol., vol. 378, p. 134687, Dec. 2025, https://doi.org/10.1016/j.seppur.2025.134687

[44] S. H. Goh, H. S. Lau, and W. F. Yong, "Metal-Organic Frameworks (MOFs)-Based Mixed Matrix Membranes (MMMs) for Gas Separation: A Review on Advanced Materials in Harsh Environmental Applications," Small, vol. 18, no. 20, p. 2107536, May 2022, https://doi.org/10.1002/smll.202107536

[45] H. Lin and B. D. Freeman, "Materials selection guidelines for membranes that remove CO2 from gas mixtures," J. Mol. Struct., vol. 739, no. 1-3, pp. 57-74, Apr. 2005, https://doi.org/10.1016/j.molstruc.2004.07.045

[46] G. Saeed et al., "Two-dimensional (2D) material nanofiltration membranes for effective recovery of lithium," Journal of Industrial and Engineering Chemistry, vol. 150, pp. 116-133, Oct. 2025, https://doi.org/10.1016/j.jiec.2025.03.004

[47] S. Pu et al., "Graphene-based nanofiltration membranes for bio-effluents downstream processing," Journal of Water Process Engineering, vol. 81, p. 109259, Jan. 2026, https://doi.org/10.1016/j.jwpe.2025.109259

[48] S. Ashtiani et al., "Metal-Organic Framework-Enabled Mixed Matrix Membranes: Recent Breakthroughs, Limitations, and Interfacial Engineering for Gas Separation," Journal of Membrane Science Letters, vol. 6, no. 1, p. 100113, Jun. 2026, https://doi.org/10.1016/j.memlet.2026.100113

[49] H. Wang, S. He, X. Qin, C. Li, and T. Li, "Interfacial Engineering in Metal-Organic Framework-Based Mixed Matrix Membranes Using Covalently Grafted Polyimide Brushes," J. Am. Chem. Soc., vol. 140, no. 49, pp. 17203-17210, Dec. 2018, https://doi.org/10.1021/jacs.8b10138

[50] H. Wei, H. Nong, L. Chen, and S. Zhang, "Advanced Materials-Based Nanofiltration Membranes for Efficient Removal of Organic Micropollutants in Water and Wastewater Treatment," Membranes 2025, Vol. 15, Page 236, vol. 15, no. 8, p. 236, Aug. 2025, https://doi.org/10.3390/membranes15080236

[51] S. Khanlari, M. A. Tofighy, and T. Mohammadi, "Transport phenomena through nanocomposite membranes," Nanocomposite Membranes for Water and Gas Separation, pp. 91-112, Jan. 2020, https://doi.org/10.1016/B978-0-12-816710-6.00004-3

[52] K. Lei et al., "Mechanochemical processing of interface-integrated mixed-matrix membranes for efficient gas separation," J. Mater. Chem. A Mater., vol. 13, no. 29, pp. 23795-23804, Jul. 2025, https://doi.org/10.1039/D5TA03665H

[53] C. Bhuyan, P. Bora, P. Rajguru, P. Gogoi, and S. Hazarika, "2D nanomaterial enabled next generation membranes for advanced water treatment," Desalination, vol. 631, p. 120177, Aug. 2026, https://doi.org/10.1016/j.desal.2026.120177

[54] M. J. Moreno and K. Balashev, "Interfacial Interactions of Nanoparticles and Molecular Nanostructures with Model Membrane Systems: Mechanisms, Methods, and Applications," Membranes 2026, Vol. 16, Page 134, vol. 16, no. 4, p. 134, Apr. 2026, https://doi.org/10.3390/membranes16040134

[55] B. Zornoza et al., "Functionalized flexible MOFs as fillers in mixed matrix membranes for highly selective separation of CO2 from CH4 at elevated pressures," Chemical Communications, vol. 47, no. 33, pp. 9522-9524, Aug. 2011, https://doi.org/10.1039/c1cc13431k

[56] B. H. Jeong et al., "Interfacial polymerization of thin film nanocomposites: A new concept for reverse osmosis membranes," J. Memb. Sci., vol. 294, no. 1-2, pp. 1-7, May 2007, https://doi.org/10.1016/j.memsci.2007.02.025

[57] Y. Zhao et al., "Metal-organic framework based membranes for selective separation of target ions," J. Memb. Sci., vol. 634, p. 119407, Sep. 2021, https://doi.org/10.1016/j.memsci.2021.119407

[58] T. H. Lee et al., "Interface engineering in MOF/crosslinked polyimide mixed matrix membranes for enhanced propylene/propane separation performance and plasticization resistance," J. Memb. Sci., vol. 667, p. 121182, Feb. 2023, https://doi.org/10.1016/j.memsci.2022.121182

[59] G. Chen, H. Zhu, G. Liu, G. Liu, and W. Jin, "Confinement Effects and Manipulation Strategies of Nanocomposite Membranes towards Molecular Separation," Angew. Chem. Int. Ed., vol. 64, no. 4, p. e202418649, Jan. 2025, https://doi.org/10.1002/anie.202418649

[60] K. Boussu, B. Van Der Bruggen, A. Volodin, J. Snauwaert, C. Van Haesendonck, and C. Vandecasteele, "Roughness and hydrophobicity studies of nanofiltration membranes using different modes of AFM," J. Colloid Interface Sci., vol. 286, no. 2, pp. 632-638, Jun. 2005, https://doi.org/10.1016/j.jcis.2005.01.095

[61] M. Samari, S. Zinadini, and A. A. Zinatizadeh, "Performance evaluation of amino-functionalized mesoporous/PES nanofiltration membrane in anionic dye removal from aqueous solutions," Appl. Water Sci., vol. 12, p. 263, 2022, https://doi.org/10.1007/s13201-022-01775-4

[62] W. Cheng, Q. Zhao, H. Chu, X. Zhou, Y. Zhang, and T. S. Chung, "Molecular innovations in nanofiltration via interfacial polymerization: from monomer design to membrane performance," Chem. Soc. Rev., vol. 55, no. 6, pp. 3380-3431, Mar. 2026, https://doi.org/10.1039/D5CS00787A

[63] S. H. Woo, J. Park, and B. R. Min, "Relationship between permeate flux and surface roughness of membranes with similar water contact angle values," Sep. Purif. Technol., vol. 146, pp. 187-191, May 2015, https://doi.org/10.1016/j.seppur.2015.03.048

[64] D. Lee, Y. J. Cha, Y. Baek, S. Choi, and Y. Lee, "Relationships among Permeability, Membrane Roughness, and Eukaryote Inhabitation during Submerged Gravity-Driven Membrane (GDM) Filtration," Appl. Sci., vol. 10, no. 22, p. 8111, 2020,https: // doi.org/10.3390/app10228111

[65] K. Tang et al., "Regulating the thickness of nanofiltration membranes for efficient water purification," Nanoscale Adv., vol. 5, no. 18, pp. 4770-4781, Sep. 2023, https://doi.org/10.1039/D3NA00110E

[66] H. Zhu, A. Szymczyk, and A. Ghoufi, "Multiscale modelling of transport in polymer-based reverse-osmosis/nanofiltration membranes: present and future," Discover Nano 2024 19:1, vol. 19, no. 1, pp. 91-, May 2024, https://doi.org/10.1186/s11671-024-04020-w

[67] T. Oyegoke, "Mitigating Environmental Risks: Efficient Removal of Metronidazole from Pharmaceutical Wastewater Using Functionalized Graphene Membrane," Engineering Proceedings, vol. 87, no. 1, p. 1, 2025, https://doi.org/10.3390/engproc2025087001

[68] O. I. Ayeni and T. Oyegoke, "Computational insights into graphene-based materials for arsenic removal from wastewater: a hybrid quantum mechanical study," Discover Water, vol. 4, no. 1, p. 103, Nov. 2024, https://doi.org/10.1007/s43832-024-00160-3

[69] O. I. Ayeni and T. Oyegoke, "Insights on Metal Doped Graphene in the Adsorption of Arsenic via DFT Calculations," Chemistry Journal of Moldova, vol. 20, no. 1, pp. 86-94, 2025, https://doi.org/10.19261/cjm.2025.1264

[70] J. P. K. Abal, R. F. Dillenburg, M. H. Köhler, and M. C. Barbosa, "Molecular Dynamics Simulations of Water Anchored in Multilayered Nanoporous MoS2 Membranes: Implications for Desalination," ACS Appl. Nano Mater., vol. 4, no. 10, pp. 10467-10476, Oct. 2021, https://doi.org/10.1021/acsanm.1c01982

[71] W. Shi, C. Xu, J. Cai, and S. Wu, "Advancements in material selection and application research for mixed matrix membranes in water treatment," J. Environ. Chem. Eng., vol. 11, no. 6, p. 111292, Dec. 2023, https://doi.org/10.1016/j.jece.2023.111292

[72] R. Wang and S. Lin, "Pore model for nanofiltration: History, theoretical framework, key predictions, limitations, and prospects," J. Memb. Sci., vol. 620, p. 118809, Feb. 2021, https://doi.org/10.1016/j.memsci.2020.118809

[73] P. M. Biesheuvel, S. Porada, B. Blankert, I. Ryzhkov, and M. Elimelech, "Analysis of concentration polarization in reverse osmosis and nanofiltration: zero-, one-, and two-dimensional models," Jan. 2024, Accessed: May 02, 2026. [Online]. Available: https://arxiv.org/pdf/2401.11527

[74] J. R. Werber, C. O. Osuji, and M. Elimelech, "Materials for next-generation desalination and water purification membranes," Nat. Rev. Mater., vol. 1, no. 5, pp. 16018-, Apr. 2016, https://doi.org/10.1038/natrevmats.2016.18

[75] A. G. Fane, R. Wang, and M. X. Hu, "Synthetic membranes for water purification: Status and future," Angew. Chem. Int. Ed., vol. 54, no. 11, pp. 3368-3386, Mar. 2015, https://doi.org/10.1002/anie.201409783

[76] D. S. Sholl and R. P. Lively, "Seven chemical separations to change the world," Nature 2016 532:7600, vol. 532, no. 7600, pp. 435-437, Apr. 2016, https://doi.org/10.1038/532435a

[77] N. Artrith et al., "Best practices in machine learning for chemistry," Nature Chemistry 2021 13:6, vol. 13, no. 6, pp. 505-508, May 2021, https://doi.org/10.1038/s41557-021-00716-z

[78] A. Tayyebi, A. S. Alshami, X. Yu, and E. Kolodka, "Can machine learning methods guide gas separation membranes fabrication?," Journal of Membrane Science Letters, vol. 2, no. 2, p. 100033, Nov. 2022, https://doi.org/10.1016/j.memlet.2022.100033

[79] Dangayach, R., Jeong, N., Demirel, E., Uzal, N., Fung, V., & Chen, Y. (2025). Machine Learning-Aided Inverse Design and Discovery of Novel Polymeric Materials for Membrane Separation. Environmental Science & Technology, 59(2), 993–1012. https://doi.org/10.1021/acs.est.4c08298

[80] Wang, H., Zeinali Danalou, S., Zhu, J., Sulimro, K., Lim, C., Basak, S., Tai, A., Siriwardana, U., Hattrick-Simpers, J., & Werber, J. R. (2026). *Developing and Validating a High-Throughput Robotic System for the Accelerated Development of Porous Membranes.* Journal of Membrane Science, 738, 124804. https://doi.org/10.1016/j.memsci.2025.124804

[81] Barnett, J. W., Bilchak, C. R., Wang, Y., Benicewicz, B. C., Murdock, L. A., Bereau, T., & Kumar, S. K. (2020). *Designing Exceptional Gas-Separation Polymer Membranes Using Machine Learning.* Science Advances, 6(20), eaaz4301. https://doi.org/10.1126/sciadv.aaz4301

[82] Hu, A., Liu, Y., Wang, X., Xia, S., & Van der Bruggen, B. (2025). *A Machine Learning Based Framework to Tailor Properties of Nanofiltration and Reverse Osmosis Membranes for Targeted Removal of Organic Micropollutants.* Water Research, 268, 122677. https://doi.org/10.1016/j.watres.2024.122677

[83] Boland, C. M., Nguyen, N. Q., & Boase, N. R. B. (2026). *Active Learning for the Discovery of Antiviral Polymers.* Macromolecular Rapid Communications, 47(8), e00890. https://doi.org/10.1002/marc.202500890

[84] X. Li et al., "Sequential closed-loop Bayesian optimization as a guide for organic molecular metallophotocatalyst formulation discovery," Nature Chemistry 2024 16:8, vol. 16, no. 8, pp. 1286-1294, Jun. 2024, https://doi.org/10.1038/s41557-024-01546-5

[85] A. V. Ponce-Bobadilla, V. Schmitt, C. S. Maier, S. Mensing, and S. Stodtmann, "Practical guide to SHAP analysis: Explaining supervised machine learning model predictions in drug development," Clin. Transl. Sci., vol. 17, no. 11, Nov. 2024, https://doi.org/10.1111/cts.70056

[86] B. Bhhatarai, W. P. Walters, C. E. C. A. Hop, G. Lanza, and S. Ekins, "Opportunities and challenges using artificial intelligence in ADME/Tox," Nat. Mater., vol. 18, no. 5, pp. 418-422, May 2019, https://doi.org/10.1038/s41563-019-0332-5

[87] C. Wang et al., "Machine learning for layer-by-layer nanofiltration membrane performance prediction and polymer candidate exploration," Chemosphere, vol. 350, p. 140999, Feb. 2024, https://doi.org/10.1016/j.chemosphere.2023.140999

[88] J. L. G. Rosa, "Artificial Neural Networks - Models and Applications," Artificial Neural Networks - Models and Applications, Oct. 2016, https://doi.org/10.5772/61493

[89] D. J. Livingstone, Ed., "Artificial Neural Networks," vol. 458, 2009, https://doi.org/10.1007/978-1-60327-101-1

[90] Q. Liu, S. Wu, L. Wang, and T. Tan, "Predicting the Next Location: A Recurrent Model with Spatial and Temporal Contexts," Proceedings of the AAAI Conference on Artificial Intelligence, vol. 30, no. 1, pp. 194-200, Feb. 2016, https://doi.org/10.1609/aaai.v30i1.9971

[91] S. Jiang, A. B. Dieng, and M. A. Webb, "Property-guided generation of complex polymer topologies using variational autoencoders," npj Computational Materials 2024 10:1, vol. 10, no. 1, pp. 139-, Jun. 2024, https://doi.org/10.1038/s41524-024-01328-0

[92] G. Liu, E. Inae, and M. Jiang, "Deep Learning for Polymer Discovery," 2026, https://doi.org/10.1007/978-3-031-84732-5

[93] S. Cuomo, V. S. Di Cola, F. Giampaolo, G. Rozza, M. Raissi, and F. Piccialli, "Scientific Machine Learning Through Physics-Informed Neural Networks: Where we are and What's Next," Journal of Scientific Computing 2022 92:3, vol. 92, no. 3, pp. 88-, Jul. 2022, https://doi.org/10.1007/s10915-022-01939-z

[94] Z. Wu, H. Zhang, H. Ye, H. Zhang, Y. Zheng, and X. Guo, "PINN enhanced extended multiscale finite element method for fast mechanical analysis of heterogeneous materials," Acta Mechanica 2024 235:7, vol. 235, no. 7, pp. 4895-4913, May 2024, https://doi.org/10.1007/s00707-024-03984-1

[95] S. Xiao, R. Hu, Z. Li, S. Attarian, K. M. Björk, and A. Lendasse, "A machine-learning-enhanced hierarchical multiscale method for bridging from molecular dynamics to continua," Neural Comput. Appl., vol. 32, no. 18, pp. 14359-14373, Sep. 2020, https://doi.org/10.1007/s00521-019-04480-7

[96] A. I. Osman et al., "Machine learning for membrane design in energy production, gas separation, and water treatment: a review," Environmental Chemistry Letters 2024 22:2, vol. 22, no. 2, pp. 505-560, Feb. 2024, https://doi.org/10.1007/s10311-023-01695-y

[97] S. Pilon et al., "A flexible and affordable self-driving laboratory for automated reaction optimization," Nature Synthesis 2026, pp. 1-13, Apr. 2026, https://doi.org/10.1038/s44160-026-01053-0

[98] A. B. Bereketoglu, "Composite Reward Design in PPO-Driven Adaptive Filtering," May 2025, Accessed: May 03, 2026. [Online]. Available: https://arxiv.org/pdf/2506.06323

[99] Q. Ai, F. Meng, J. Shi, B. Pelkie, and C. W. Coley, "Extracting structured data from organic synthesis procedures using a fine-tuned large language model," Digital Discovery, vol. 3, no. 9, pp. 1822-1831, Sep. 2024, https://doi.org/10.1039/D4DD00091A

[100] A. M. Mroz et al., "Cross-disciplinary perspectives on the potential for artificial intelligence across chemistry," Chem. Soc. Rev., vol. 54, no. 11, pp. 5433-5469, Jun. 2025, https://doi.org/10.1039/D5CS00146C

[101] F. van Rooij, P. Scarf, and P. Do, "Planning the restoration of membranes in RO desalination using a digital twin," Desalination, vol. 519, p. 115214, Dec. 2021, https://doi.org/10.1016/j.desal.2021.115214

[102] M. ; Rosenfeld et al., "Methodology for the Development of Virtual Representations within the Process Development Framework of Energy Plants: From Digital Model to Digital Predictive Twin-A Review," Energies 2023, Vol. 16, Page 2641, vol. 16, no. 6, p. 2641, Mar. 2023, https://doi.org/10.3390/en16062641

[103] Y. Benchenina, A. Zemmit, and M. M. Bouzaki, "Enhancing fuel cell efficiency through advanced digital twin modelling," STUDIES IN ENGINEERING AND EXACT SCIENCES, vol. 5, no. 1, pp. 2102-2114, May 2024, https://doi.org/10.54021/seesv5n1-104

[104] O. A. Prado-Rubio, W. F. Hui, M. Stevnsborg, M. Pinelo, and J. K. Huusom, "Digital-twin development for a novel vibrating membrane aiming at fractionating fermentation broths," Computer Aided Chemical Engineering, vol. 52, pp. 2575-2580, Jan. 2023, https://doi.org/10.1016/B978-0-443-15274-0.50409-1

[105] W. J. Lau and A. F. Ismail, "Polymeric nanofiltration membranes for textile dye wastewater treatment: Preparation, performance evaluation, transport modelling, and fouling control - a review," Desalination, vol. 245, no. 1-3, pp. 321-348, Sep. 2009, https://doi.org/10.1016/j.desal.2007.12.058

[106] K. Boussu et al., "Characterization of polymeric nanofiltration membranes for systematic analysis of membrane performance," J. Memb. Sci., vol. 278, no. 1-2, pp. 418-427, Jul. 2006, https://doi.org/10.1016/j.memsci.2005.11.027

[107] T. Shibutani et al., "Membrane fouling properties of hollow fibre membranes prepared from cellulose acetate derivatives," J. Memb. Sci., vol. 376, no. 1-2, pp. 102-109, Jul. 2011, https://doi.org/10.1016/j.memsci.2011.04.006

[108] S. Zinadini, S. Rostami, V. Vatanpour, and E. Jalilian, "Preparation of antibiofouling polyethersulfone mixed matrix NF membrane using photocatalytic activity of ZnO/MWCNTs nanocomposite," J. Memb. Sci., vol. 529, pp. 133-141, May 2017, https://doi.org/10.1016/j.memsci.2017.01.047

[109] C. Alvarado, K. Farris, and J. Kilduff, "Membrane Fouling, Modelling and Recent Developments for Mitigation," Emerging Membrane Technology for Sustainable Water Treatment, pp. 433-462, Mar. 2016, https://doi.org/10.1016/B978-0-444-63312-5.00017-6

[110] W. Ye et al., "Theoretical and experimental study of organic fouling of loose nanofiltration membrane," J. Taiwan Inst. Chem. Eng., vol. 93, pp. 509-518, Dec. 2018, https://doi.org/10.1016/j.jtice.2018.08.029

[111] M. R. Esfahani, H. A. Stretz, and M. J. M. Wells, "Comparing humic acid and protein fouling on polysulfone ultrafiltration membranes: Adsorption and reversibility," Journal of Water Process Engineering, vol. 6, pp. 83-92, Jun. 2015, https://doi.org/10.1016/j.jwpe.2015.03.001

[112] M. A. Sari and S. Chellam, "Relative contributions of organic and inorganic fouling during nanofiltration of inland brackish surface water," J. Memb. Sci., vol. 523, pp. 68-76, Feb. 2017, https://doi.org/10.1016/j.memsci.2016.10.005

[113] O. Habimana, A. J. C. Semião, and E. Casey, "The role of cell-surface interactions in bacterial initial adhesion and consequent biofilm formation on nanofiltration/reverse osmosis membranes," J. Memb. Sci., vol. 454, pp. 82-96, Mar. 2014, https://doi.org/10.1016/j.memsci.2013.11.043

[114] R. Heu, M. Ateia, and C. Yoshimura, "Photocatalytic Nanofiltration Membrane Using Zr-MOF/GO Nanocomposite with High-Flux and Anti-Fouling Properties," Catalysts 2020, Vol. 10, Page 711, vol. 10, no. 6, p. 711, Jun. 2020, https://doi.org/10.3390/catal10060711

[115] Y. Li, Y. J. Zhao, M. Wang, and H. Y. Wang, "Enhanced anti-fouling and selective performance of GO-modified nanofiltration membranes for lithium extraction from salt lake brine," Chemical Engineering Journal, vol. 499, p. 156269, Nov. 2024, https://doi.org/10.1016/j.cej.2024.156269

[116] T. Yan et al., "A critical review on membrane hybrid system for nutrient recovery from wastewater," Chemical Engineering Journal, vol. 348, pp. 143-156, Sep. 2018, https://doi.org/10.1016/j.cej.2018.04.166

[117] J. Wang, Z. Wang, Y. Liu, J. Wang, and S. Wang, "Surface modification of NF membrane with zwitterionic polymer to improve anti-biofouling property," J. Memb. Sci., vol. 514, pp. 407-417, Sep. 2016, https://doi.org/10.1016/j.memsci.2016.05.014

[118] X. Wang et al., "Highly efficient nanofibrous sterile membrane with anti-BSA/RNA-fouling surface via plasma-assisted carboxylation process," J. Memb. Sci., vol. 601, p. 117935, Mar. 2020, https://doi.org/10.1016/j.memsci.2020.117935

[119] G. Muhammad, H. Nagasawa, T. Hamura, N. Moriyama, T. Tsuru, and M. Kanezashi, "Fabrication of Nanoporous Silica Membranes by Atmospheric-Pressure Plasma-Enhanced Chemical Vapor Deposition Using Porogen Approach," Chem. Asian J., vol. 21, no. 2, p. e00948, Jan. 2026, https://doi.org/10.1002/asia.202500948

[120] A. Y. Bagastyo, A. D. Anggrainy, C. S. Nindita, and Warmadewanthi, "Electrodialytic removal of fluoride and calcium ions to recover phosphate from fertilizer industry wastewater," Sustainable Environment Research, vol. 27, no. 5, pp. 230-237, Sep. 2017, https://doi.org/10.1016/j.serj.2017.06.002

[121] "Membranes Market Report 2025-2030 [257 Pages & 270 Tables], Market Size." Accessed: May 03, 2026. https://w ww. mark e tsandmarkets.com/Market-Reports/membranes-market-1176.html

[122] W. A. Khattak, M. Anas, E. E. Hakki, J. Iqbal, B. A. Abbasi, and A. Munir, "Economical and Societal Debut on Sustainable Environment and Industry Using Bioenergy and Nanotechnology," pp. 191-219, 2026, https://doi.org/10.1007/978-981-95-5875-9_10

[123] Giulia Mancò, Umberto Tesio, Elisa Guelpa, Vittorio Verda, A review on multi energy systems modelling and optimization, Applied Thermal Engineering, Volume 236, Part E, 2024, 121871, ISSN 1359-4311, https://doi.org/ 10.1016 /j. applthermaleng.2023.121871

[124] Prashant Nagapurkar, Kiran Thirumaran, Michelle K. Kidder, Techno-economic and environmental life cycle assessment of next-generation fiber-encapsulated nanoscale hybrid materials for direct air carbon capture, Sustainable Materials and Technologies, Volume 39, 2024, e00803,ISSN 2214-9937, https://doi.org/10.1016/j.susmat.2023.e00803

[125] L. Äkräs, F. Silvenius, H. Baniasadi, M. Vahvaselkä, H. Ilvesniemi, and J. Seppälä, "A cradle-to-gate life cycle assessment of polyamide-starch biocomposites: carbon footprint as an indicator of sustainability," Clean Technologies and Environmental Policy 2024 26:10, vol. 26, no. 10, pp. 3297-3312, May 2024, https://doi.org/10.1007/s10098-024-02884-1

[126] T. Krahnstöver, R. Hochstrat, and T. Wintgens, "Comparison of methods to assess the integrity and separation efficiency of ultrafiltration membranes in wastewater reclamation processes," J. Water Process Eng., vol. 30, p. 100646, Aug. 2019, https://doi.org/10.1016/J.JWPE.2018.06.008

[127] P. Karka, S. Papadokonstantakis, and A. Kokossis, "Cradle-to-gate assessment of environmental impacts for a broad set of biomass-to-product process chains," The International Journal of Life Cycle Assessment 2017 22:9, vol. 22, no. 9, pp. 1418-1440, Feb. 2017, https://doi.org/10.1007/s11367-017-1262-6

[128] T. Srebotnjak, "Cradle-to-Grave and Sustainable Development," Encyclopedia of Sustainability in Higher Education, pp. 331-334, Jan. 2019, https://doi.org/10.1007/978-3-030-11352-0_274

[129] A. Accardo, G. Dotelli, F. Miretti, and E. Spessa, "End-of-Life Impact on the Cradle-to-Grave LCA of Light-Duty Commercial Vehicles in Europe," Applied Sciences (Switzerland), vol. 13, no. 3, p. 1494, Feb. 2023, https://doi.org/10.3390/app13031494

[130] N. Attari and R. Hausler, "Cradle-to-Gate Life Cycle Assessment of Cellulose-Based Membrane Manufacturing Process," International Journal of Environmental Pollution and Remediation, vol. 11, pp. 20-31, 2023, https://doi.org/10.11159 /ijepr. 2023.003

[131] P. Yadav, N. Ismail, M. Essalhi, M. Tysklind, D. Athanassiadis, and N. Tavajohi, "Assessment of the environmental impact of polymeric membrane production," J. Memb. Sci., vol. 622, p. 118987, Mar. 2021, https://doi.org/10.1016/ j.memsci .2020. 118987

[132] C. Y. Loh, A. D. Burrows, and M. Xie, "Sustainable Polymeric Membranes: Green Chemistry and Circular Economy Approaches," ACS ES&T Engineering, vol. 5, no. 8, pp. 1882-1906, Aug. 2025, https://doi.org/10.1021/acsestengg.5c00282

[133] R. A. Ibrahim, H. Inan, and I. S. Fahim, "A comparative cradle-to-gate life cycle assessment of three cotton stalk waste sustainable applications," Scientific Reports 2023 13:1, vol. 13, no. 1, pp. 20781-, Nov. 2023, https://doi.org/10.1038/s41598-023-47817-y

[134] Wahiduzzaman, M. R. Khan, S. Harp, J. Neumann, and Q. N. Sultana, "Processing and Performance of MOF (Metal Organic Framework)-Loaded PAN Nanofibrous Membrane for CO2 Adsorption," Journal of Materials Engineering and Performance 2016 25:4, vol. 25, no. 4, pp. 1276-1283, Feb. 2016, https://doi.org/10.1007/s11665-016-1966-y

[135] S. Dutta, M. Walden, A. Sinelshchikova, R. Ettlinger, E. Lizundia, and S. Wuttke, "Cradle-to-Gate Environmental Impact Assessment of Commercially Available Metal-Organic Frameworks Manufacturing," Adv. Funct. Mater., vol. 34, no. 52, p. 2410751, Dec. 2024, https://doi.org/10.1002/adfm.202410751

[136] P. Singh, S. Panwar, and P. N. Dave, "Advancing Environmental Remediation with Metal-Organic Frameworks: Perspectives on Green Synthesis, Scale-Up Strategies, Techno-Economic Analysis, and Life Cycle Assessment," Adv. Mater. Technol., vol. 11, no. 3, p. e01309, Feb. 2026, https://doi.org/10.1002/admt.202501309

[137] F. Bahmei, N. Bahramifar, S. Ghasemi, H. Younesi, and M. Weil, "Comparison of environmental impacts in the production of graphene from biomass waste and the Hummers' method," J. Clean. Prod., vol. 497, p. 145145, Mar. 2025, https://doi.org/10.1016/j.jclepro.2025.145145

[138] A. Al-Amiery, W. N. R. W. Isahak, A. Al-Amiery, and W. N. R. W. Isahak, "Graphene for a Sustainable Future: Clean Energy, Environmental Remediation, and Green Pathways a Review," Terra Joule J., vol. 2, no. 1, p. 8, Mar. 2026, https://doi.org/10.64071/3080-5724.1029

[139] S. Dini, A. E. D. A. Bekhit, S. Roohinejad, J. M. Vale, and D. Agyei, "The Physicochemical and Functional Properties of Biosurfactants: A Review," Molecules, vol. 29, no. 11, p. 2544, May 2024, https://doi.org/10.3390/MOLECULES29112544

[140] Z. Wang et al., "Closed-Loop Recycling of End-of-Life Poly (Ether Sulfone) Membranes: Upcycling Waste into Bisphenol S via a Catalyst-Free Hydrolysis Process," Environ. Sci. Technol., vol. 60, no. 15, pp. 11787–11796, 2026, https://doi.org/10.1021/acs.est.6c03085.

[141] I. P. da Silva et al., "Transfiguration of discarded PVDF ultrafiltration membranes: Optimization of pyrolysis parameters for high-value char production," Waste Manage., vol. 190, pp. 360–369, Nov. 2024, https://doi.org/10.1016/j.wasman. 2024.09.033.

[142] S.-R. Kim et al., "Toward Microcapsule-Embedded Self-Healing Membranes," Environ. Sci. Technol. Lett., vol. 3, no. 5, pp. 216–221, May 2016, https://doi.org/10.1021/acs.estlett.6b00046.

[143] M. El-Bagoury, D. Aboelela, M. Alyoubi, and S. M. S. Abdel-Hamid, "Economic and Environmental Aspects," Water Treatment and Desalination: Membrane Separation using Renewable Energy Resources, pp. 399-423, Jan. 2025,https://doi.org/10.1002/9781394300105.CH13

[144] P. Gajjar and S. Koyani, "MEMBRANE TECHNOLOGY FOR LOW-COST SMALL WATER TREATMENT IN DEVELOPING COUNTRIES," INTERNATIONAL JOURNAL OF CIVIL ENGINEERING AND TECHNOLOGY (IJCIET), vol. 16, no. 4, pp. 1-19, Jul. 2025, https://doi.org/10.34218/IJCIET_16_04_001

[145] E. A. Iyiegbuniwe, U. U. Nwosu, and S. Kodali, "A Review of Occupational Health Implications of Exposure and Risk Management of Carbon Nanotubes and Carbon Nanofibres," International Journal of Environmental Science and Development, vol. 7, no. 11, pp. 849-855, 2016, https://doi.org/10.18178/ijesd.2016.7.11.893

[146] M. Lippmann, "Toxicological and epidemiological studies on effects of airborne fibres: Coherence and public health implications," Crit. Rev. Toxicol., vol. 44, no. 8, pp. 643-695, 2014, https://doi.org/10.3109/10408444.2014.928266

[147] A. R. Elasaly and J. Bogacki, "Application of multi-criteria analysis for selecting the most sustainable industrial wastewater treatment technology," Cleaner Water, vol. 5, p. 100225, Mar. 2026, https://doi.org/10.1016/j.clwat.2026.100225

[148] B. Hosseini Monjezi, K. Kutonova, M. Tsotsalas, S. Henke, and A. Knebel, "Current Trends in Metal-Organic and Covalent Organic Framework Membrane Materials," Angew. Chem. Int. Ed., vol. 60, no. 28, pp. 15153-15164, Jul. 2021, https://doi.org/10.1002/anie.202015790

[149] G. M. Jaid, A. A. AbdulRazak, H. Meskher, S. Al-Saadi, and Q. F. Alsalhy, "Metal-organic frameworks (MOFs), covalent organic frameworks (COFs), and hydrogen-bonded organic frameworks (HOFs) in mixed matrix membranes," Materials Today Sustainability, vol. 25, p. 100672, Mar. 2024, https://doi.org/10.1016/j.mtsust.2024.100672

[150] Z. Lin, Z. Yuan, Z. Dai, L. Shao, M. S. Eisen, and X. He, "A review from material functionalization to process feasibility on advanced mixed matrix membranes for gas separations," Chemical Engineering Journal, vol. 475, p. 146075, Nov. 2023, https://doi.org/10.1016/j.cej.2023.146075

[151] V. Muthukumaraswamy Rangaraj et al., "Metal Organic Framework - Based Mixed Matrix Membranes for Carbon Dioxide Separation: Recent Advances and Future Directions," Front. Chem., vol. 8, p. 506894, Jul. 2020, https://doi.org/10.3389 /fchem. 2020.00534

[152] S. A. Ali et al., "Review on Synthesis and Characterization of Advanced Nanomaterials-based Mixed Matrix Membranes (MMMs) for CO2 Capture: Progress, Challenges, and Prospects," Energy & Fuels, vol. 38, no. 19, pp. 18330-18366, Oct. 2024, https://doi.org/10.1021/acs.energyfuels.4c03305

[153] A. Katare, S. Kumar, S. Kundu, S. Sharma, L. M. Kundu, and B. Mandal, "Mixed Matrix Membranes for Carbon Capture and Sequestration: Challenges and Scope," ACS Omega, vol. 8, no. 20, pp. 17511-17522, May 2023, https://doi.org/10.1021/ acsomega.3c01666

[154] R. N. Tabi, P. Boakye, F. O. Agyemang, E. N. Nxumalo, and S. Oduro-Kwarteng, "A review of spiral wound membrane modules and processes for groundwater treatment," Frontiers in Membrane Science and Technology, vol. 3, p. 1343651, Apr. 2024, https://doi.org/10.3389/frmst.2024.1343651

[155] F. Rehman, K. H. Thebo, M. Aamir, and J. Akhtar, "Nanomembranes for water treatment," Nanotechnology in the Beverage Industry: Fundamentals and Applications, pp. 207-240, Jan. 2020, https://doi.org/10.1016/B978-0-12-819941-1.00008-0

[156] S. Das et al., "Assessing Advances in Anti-fouling Membranes to Improve Process Economics and Sustainability of Water Treatment," ACS ES&T Engineering, vol. 2, no. 11, pp. 2159-2173, Nov. 2022, https://doi.org/10.1021/acsestengg.2c00184

[157] A. Bilal et al., "Enhancing Water Purification by Integrating Titanium Dioxide Nanotubes into Polyethersulfone Membranes for Improved Hydrophilicity and Anti-Fouling Performance," Membranes 2024, Vol. 14, Page 116, vol. 14, no. 5, p. 116, May 2024, https://doi.org/10.3390/membranes14050116

[158] M. Maghami, A. Abdelrasoul, M. Maghami, and A. Abdelrasoul, "Zeolites-Mixed-Matrix Nanofiltration Membranes for the Next Generation of Water Purification," Nanofiltration, Jul. 2018, https://doi.org/10.5772/intechopen.75083

[159] M. A. Junker, W. M. de Vos, R. G. H. Lammertink, and J. de Grooth, "Bridging the gap between lab-scale and commercial dimensions of hollow fibre nanofiltration membranes," J. Memb. Sci., vol. 624, p. 119100, Apr. 2021, https://doi.org/10.1016/j.memsci.2021.119100

[160] K. Tang et al., "Regulating the thickness of nanofiltration membranes for efficient water purification," Nanoscale Adv., vol. 5, no. 18, pp. 4770-4781, Sep. 2023, https://doi.org/10.1039/D3NA00110E

[161] K. Yang et al., "Stretched ZIF-8@GO flake-like fillers via pre-Zn(II)-doping strategy to enhance CO2 permeation in mixed matrix membranes," J. Memb. Sci., vol. 601, p. 117934, Mar. 2020, https://doi.org/10.1016/j.memsci.2020.117934

[162] E. L. Subtil, R. Almeria Ragio, H. G. Lemos, G. Scaratti, J. García, and P. Le-Clech, "Direct membrane filtration (DMF) of municipal wastewater by mixed matrix membranes (MMMs) filled with graphene oxide (GO): Towards a circular sanitation model," Chemical Engineering Journal, vol. 441, p. 136004, Aug. 2022, https://doi.org/10.1016/j.cej.2022.136004

[163] W. A. Jonkers, E. R. Cornelissen, and W. M. de Vos, "Hollow fibre nanofiltration: From lab-scale research to full-scale applications," J. Memb. Sci., vol. 669, Mar. 2023, https://doi.org/10.1016/j.memsci.2022.121234

[164] Y. Ueda, S. Morisada, H. Kawakita, M. Wenzel, J. J. Weigand, and K. Ohto, "Effective extraction of Pt(IV) as [PtCl6]2− from hydrochloric acid using a simple urea extractant," Sep. Purif. Technol., vol. 277, Dec. 2021, https://doi.org/10.1016/j.seppur.2021.119456

[165] J. Alam et al., "Graphene oxide, an effective nanoadditive for a development of hollow fibre nanocomposite membrane with antifouling properties," Advances in Polymer Technology, vol. 37, no. 7, pp. 2597-2608, Nov. 2018, https://doi.org/ 10. 1002/adv.21935

[166] R. Patala, O. T. Mahlangu, H. Nyoni, B. B. Mamba, and A. T. Kuvarega, "In Situ Generation of Fouling Resistant Ag/Pd Modified PES Membranes for Treatment of Pharmaceutical Wastewater," Membranes 2022, Vol. 12, Page 762, vol. 12, no. 8, p. 762, Aug. 2022, https://doi.org/10.3390/membranes12080762

[167] S. Bandini and V. Morelli, "Mass transfer in 1812 spiral wound modules: Experimental study in dextrose-water nanofiltration," Sep. Purif. Technol., vol. 199, pp. 84-96, Jun. 2018, https://doi.org/10.1016/j.seppur.2018.01.044

[168] Y. Zhang, L. Zhang, L. Hou, S. Kuang, and A. Yu, "Modelling of the variations of permeate flux, concentration polarization, and solute rejection in nanofiltration system," AIChE Journal, vol. 65, no. 3, pp. 1076-1087, Mar. 2019, https://doi.org/10.1002/aic.16475

[169] S. K. A. Al-Amshawee and M. Y. B. M. Yunus, "Electrodialysis membrane with concentration polarization - A review," Chemical Engineering Research and Design, vol. 201, pp. 645-678, Jan. 2024, https://doi.org/10.1016/j.cherd.2023.10.060

[170] A. Pal et al., "Mixed-matrix membranes with enhanced antifouling activity: Probing the surface-tailoring potential of tiron and chromotropic acid for nano-Tio2," R. Soc. Open Sci., vol. 4, no. 9, Sep. 2017, https://doi.org/10.1098/rsos.170368

[171] J. Caspar, G. Xue, and A. Oztekin, "Performance characteristics on up-scaling vacuum membrane distillation modules," Desalination, vol. 569, p. 116994, Jan. 2024, https://doi.org/10.1016/j.desal.2023.116994

[172] R. Ma, B. Castro-Dominguez, A. G. Dixon, and Y. H. Ma, "Scalability of multitube membrane modules for hydrogen separation: Technical considerations, issues and solutions," J. Memb. Sci., vol. 564, pp. 887-896, Oct. 2018, https://doi.org /10 . 1016/j.memsci.2018.08.003

[173] S. Soukane et al., "Scaling sets the limits of large scale membrane distillation modules for the treatment of high salinity feeds," J. Clean. Prod., vol. 287, Mar. 2021, https://doi.org/10.1016/J.JCLEPRO.2020.125555

[174] Y. Liu et al., "Advancements in nanofiltration fouling phenomenon: From water treatment to salt lakes environments," Desalination, vol. 583, Aug. 2024, https://doi.org/10.1016/j.desal.2024.117649

[175] M. Jafari et al., "Cost of fouling in full-scale reverse osmosis and nanofiltration installations in the Netherlands," Desalination, vol. 500, Mar. 2021, https://doi.org/10.1016/j.desal.2020.114865

[176] J. Wang, C. Liu, S. Ding, and Y. Yang, "Nanofiltration (NF) application in drinking water treatment plants and the challenges of its concentrate management in China," Desalination, vol. 611, Sep. 2025, https://doi.org/10.1016/ j.desal. 2025 . 118937

[177] Y. Guo et al., "Membrane fouling in engineering nanofiltration process for drinking water treatment: The spatial and chemical aspects," J. Memb. Sci., vol. 695, p. 122491, Mar. 2024, https://doi.org/10.1016/j.memsci.2024.122491

[178] T. Siddique, S. Gangadoo, D. Quang Pham, N. K. Dutta, and N. R. Choudhury, "Antifouling and Antimicrobial Study of Nanostructured Mixed-Matrix Membranes for Arsenic Filtration," Nanomaterials 2023, Vol. 13, Page 738, vol. 13, no. 4, p. 738, Feb. 2023, https://doi.org/10.3390/nano13040738

[179] L. B. Grossi, E. F. O. Neves, L. C. Lange, and M. C. S. Amaral, "Sustainability in reverse osmosis membranes waste management: Environmental and socioeconomic assessment," Desalination, vol. 575, p. 117338, Apr. 2024, https://doi.org/10.1016/j.desal.2024.117338

[180] H. Y. N. Thi, B. T. D. Nguyen, and J. F. Kim, "Sustainable Fabrication of Organic Solvent Nanofiltration Membranes," Membranes 2021, Vol. 11, Page 19, vol. 11, no. 1, p. 19, Dec. 2020, https://doi.org/10.3390/membranes11010019

[181] R. Li, Y. Zheng, X. Zhang, M. Tan, J. Wang, and G. Tian, "Enhanced Lithium Recovery from Salt-Lake Brines via Advanced Nanofiltration Membranes: Polymeric Structure-Sieving Performance Relationships," Polymers 2025, Vol. 17, Page 1440, vol. 17, no. 11, p. 1440, May 2025, https://doi.org/10.3390/polym17111440

[182] European Parliament and Council of the European Union, "Regulation (EC) No 1907/2006 concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH)," Off. J. Eur. Union, vol. L396, pp. 1–849, Dec. 2006. [Online]. Available: https://eur-lex.europa.eu/legal-content/EN/TXT/PDF/?uri=CELEX:32006R1907

[183] International Organization for Standardization, ISO 9001:2015 — Quality management systems — Requirements, ISO, Geneva, Switzerland, 2015. [Online]. Available: https://www.iso.org/standard/62085.html

[184] International Organization for Standardization, ISO 14001:2026 — Environmental management systems — Requirements with guidance for use, ISO, Geneva, Switzerland, 2026. [Online]. Available: https://www.iso.org/standard/14001

[185] Y. Cheng et al., "Enhanced Polymer Crystallinity in Mixed-Matrix Membranes Induced by Metal-Organic Framework Nanosheets for Efficient CO2 Capture," ACS Appl. Mater. Interfaces, vol. 10, no. 49, pp. 43095-43103, Dec. 2018, https://doi.org/10.1021/acsami.8b16386

[186] S. Yu, C. Li, S. Zhao, M. Chai, J. Hou, and R. Lin, "Recent advances in the interfacial engineering of MOF-based mixed matrix membranes for gas separation," Nanoscale, vol. 16, no. 16, pp. 7716-7733, Apr. 2024, https://doi.org/10.1039/ D4NR 00096J

[187] S. Gu, L. Li, F. Liu, and J. Li, "Biochar/Kevlar Nanofibre Mixed Matrix Nanofiltration Membranes with Enhanced Dye/Salt Separation Performance," Membranes 2021, Vol. 11, Page 443, vol. 11, no. 6, p. 443, Jun. 2021, https://doi.org/10.3390 / membranes11060443

[188] N. Bashir et al., "Green-synthesized silver nanoparticle-enhanced nanofiltration mixed matrix membranes for high-performance water purification," Scientific Reports 2025 15:1, vol. 15, no. 1, pp. 1001-, Jan. 2025, https://doi.org/10.1038/ s41598-024-83801-w

[189] A. Torre-Celeizabal, C. Casado-Coterillo, and A. Garea, "Biopolymer-Based Mixed Matrix Membranes (MMMs) for CO2/CH4 Separation: Experimental and Modelling Evaluation," Membranes 2022, Vol. 12, Page 561, vol. 12, no. 6, p. 561, May 2022, https://doi.org/10.3390/membranes12060561

[190] B. Arundhathi, M. Pabba, S. S. Raj, N. Sahu, and S. Sridhar, "Advancements in Mixed-Matrix Membranes for Various Separation Applications: State of the Art and Future Prospects," Membranes 2024, Vol. 14, Page 224, vol. 14, no. 11, p. 224, Oct. 2024, https://doi.org/10.3390/membranes14110224

[191] R. Sutar and N. H. Sajal, "Gas Separation Membranes: Advances in Polymer and Mixed-Matrix Membranes for CO_2 Capture," Innovatech Engineering Journal, vol. 1, no. 01, pp. 159-176, Nov. 2024, https://doi.org/10.70937/itej.v1i01.16